Nuclear Lattice Simulations

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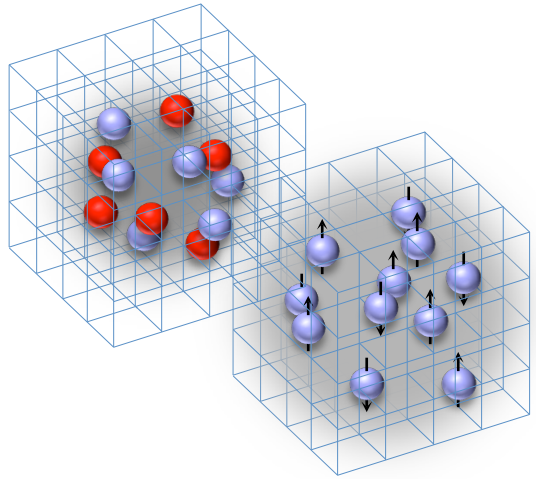


Outline

Lattice effective field theory

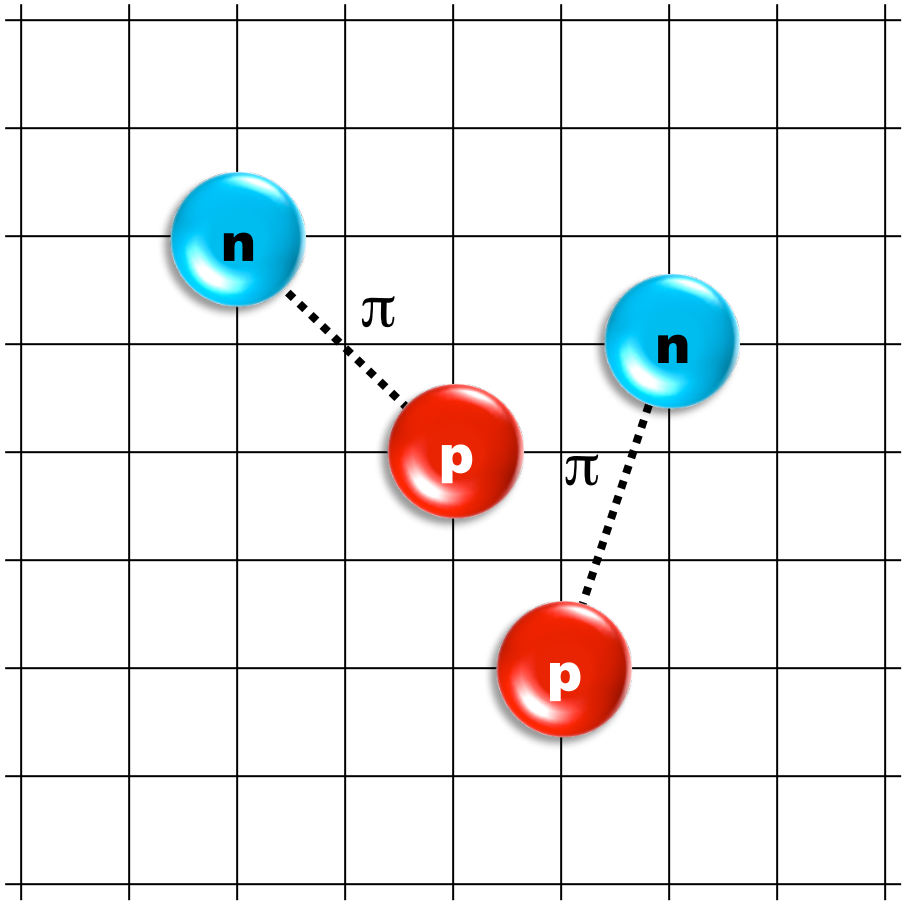
Adiabatic projection method

Pinhole algorithm

Eigenvector continuation

Summary and outlook

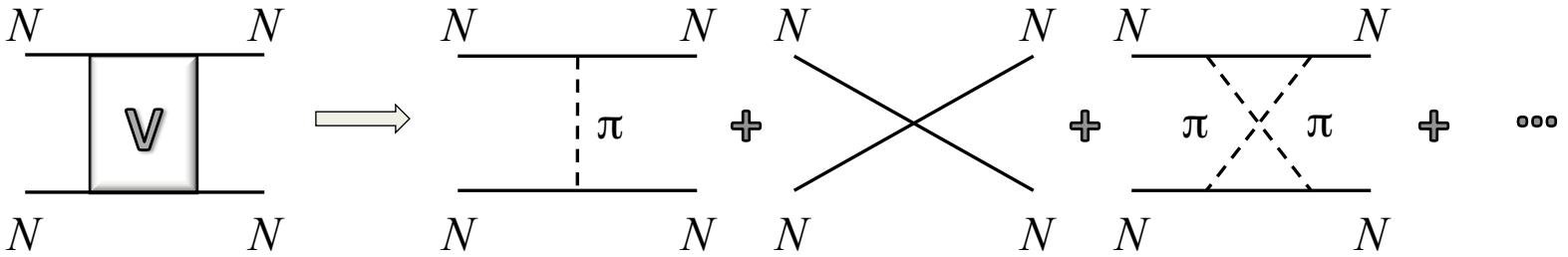
Lattice chiral effective field theory



Review: D.L, Prog. Part. Nucl. Phys. 63 117-154 (2009)
TALENT summer school lectures: qmc2016.wordpress.ncsu.edu

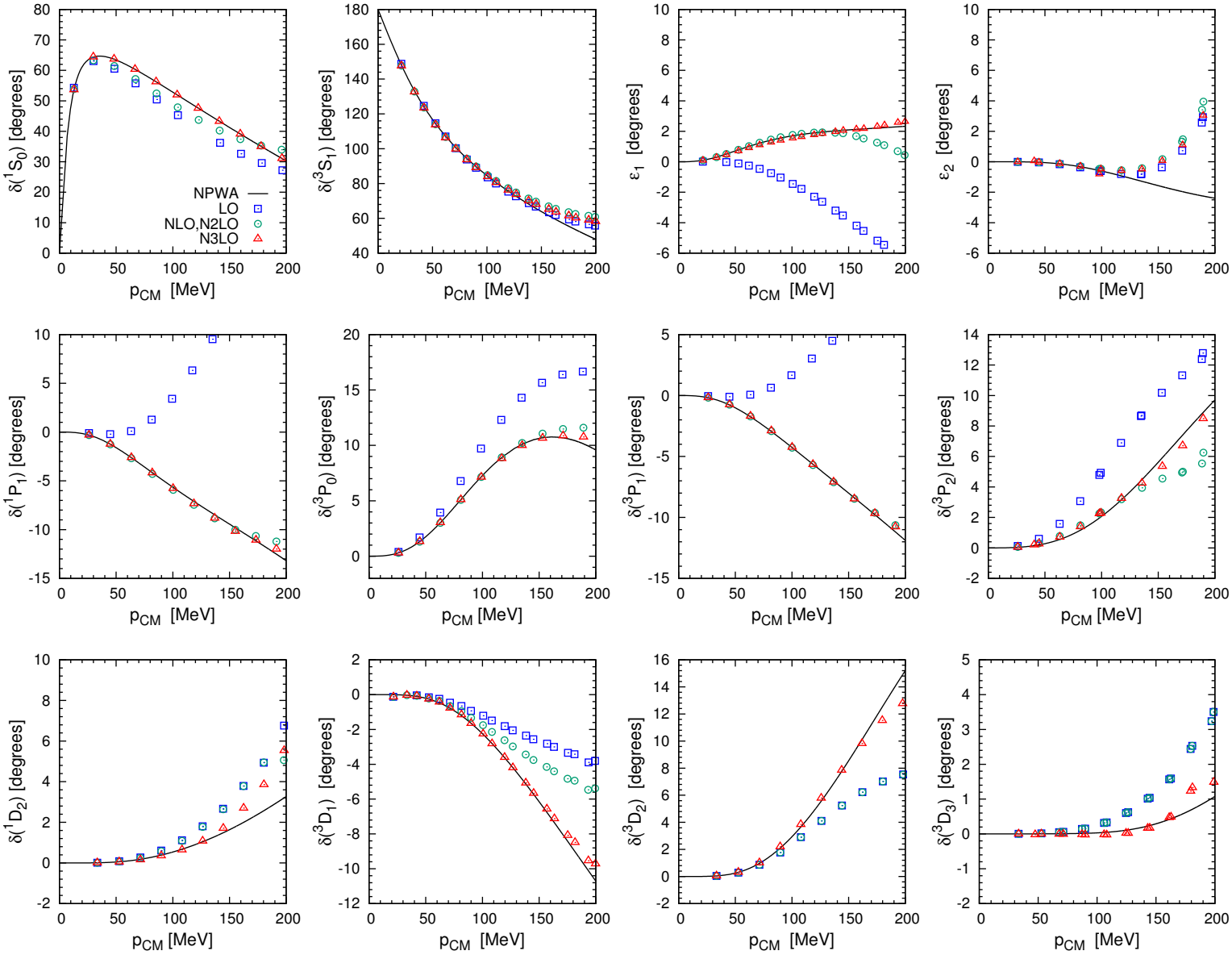
Chiral effective field theory

Construct the effective potential order by order

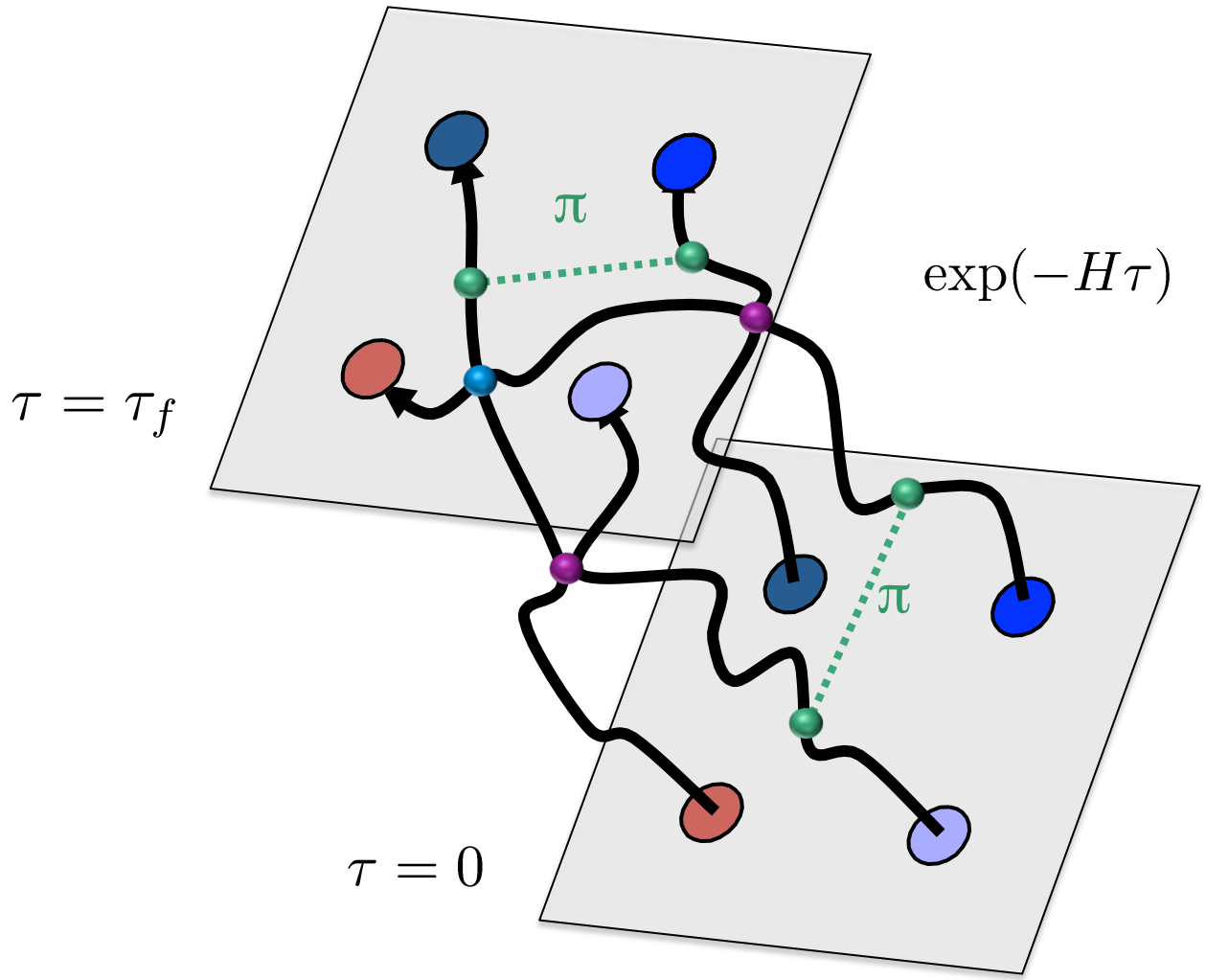


V^{OPEP} Contact interactions V^{TPEP}

Leading order (LO) Next-to-leading order (NLO)


δ(1S0) [degrees]
δ(3S1) [degrees]
ε1 [degrees]
ε2 [degrees]
δ(1P1) [degrees]
δ(3P0) [degrees]
δ(3P1) [degrees]
δ(3P2) [degrees]
δ(1D2) [degrees]
δ(3D1) [degrees]
δ(3D2) [degrees]
δ(3D3) [degrees]
pCM [MeV]
NPWA
LO
NLO,N2LO
N3LO

Euclidean time projection



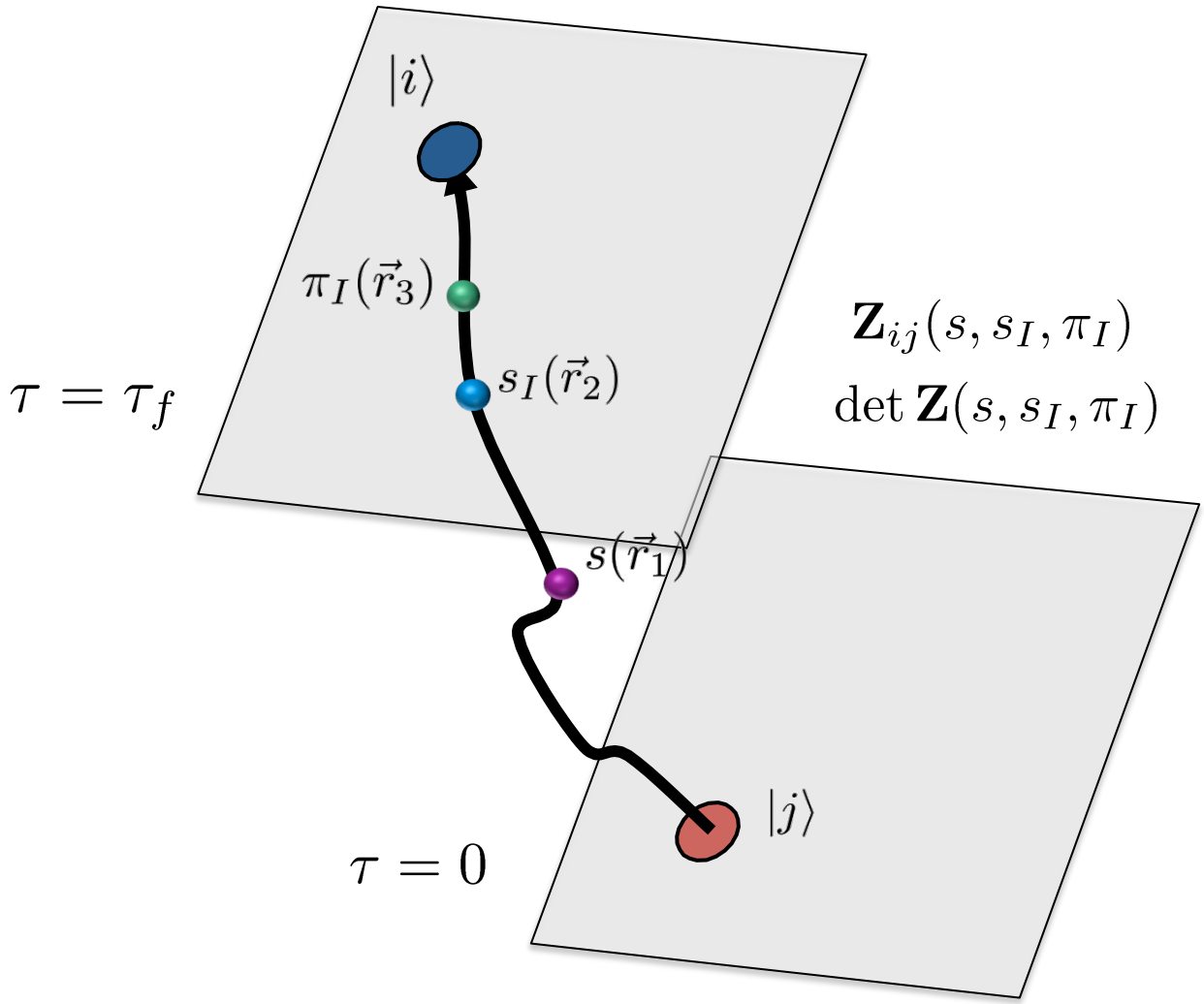
Auxiliary field method

We can write exponentials of the interaction using a Gaussian integral identity

$$\exp\left[-\frac{C}{2}(N^\dagger N)^2\right] \qquad \times \quad (N^\dagger N)^2$$

$$= \sqrt{\frac{1}{2\pi}} \int_{-\infty}^{\infty} ds \exp\left[-\frac{1}{2}s^2 + \sqrt{-C}\, s(N^\dagger N)\right] \qquad \rangle \bullet \; sN^\dagger N$$

We remove the interaction between nucleons and replace it with the interactions of each nucleon with a background field.


$|i\rangle$
$\pi_I(\vec{r}_3)$
$s_I(\vec{r}_2)$
$s(\vec{r}_1)$
$|j\rangle$
$\tau = \tau_f$
$\tau = 0$
$\mathbf{Z}_{ij}(s, s_I, \pi_I)$
$\det \mathbf{Z}(s, s_I, \pi_I)$

Science objectives

Want *ab initio* calculations of scattering and reactions relevant to alpha processes in stellar evolution and Type Ia supernovae

$^4\mathrm{He} + {}^4\mathrm{He} \rightarrow {}^4\mathrm{He} + {}^4\mathrm{He}$

$^4\mathrm{He} + {}^4\mathrm{He} + {}^4\mathrm{He} \rightarrow {}^{12}\mathrm{C} + \gamma$

$^{12}\mathrm{C} + {}^4\mathrm{He} \rightarrow {}^{16}\mathrm{O} + \gamma$

$^{16}\mathrm{O} + {}^4\mathrm{He} \rightarrow {}^{20}\mathrm{Ne} + \gamma$

$^{20}\mathrm{Ne} + {}^4\mathrm{He} \rightarrow {}^{24}\mathrm{Mg} + \gamma$

$^{24}\mathrm{Mg} + {}^4\mathrm{He} \rightarrow {}^{28}\mathrm{Si} + \gamma$

$^{12}\mathrm{C} + {}^{12}\mathrm{C} \rightarrow {}^{20}\mathrm{Ne} + {}^4\mathrm{He}$

$^{16}\mathrm{O} + {}^{16}\mathrm{O} \rightarrow {}^{28}\mathrm{Si} + {}^4\mathrm{He}$

Challenge

How to reduce the computational scaling of the calculations with number of nucleons?

Adiabatic projection method

The adiabatic projection method is a first principles method for scattering and reactions. It computes enough scattering information from Monte Carlo simulations to construct an effective Hamiltonian.

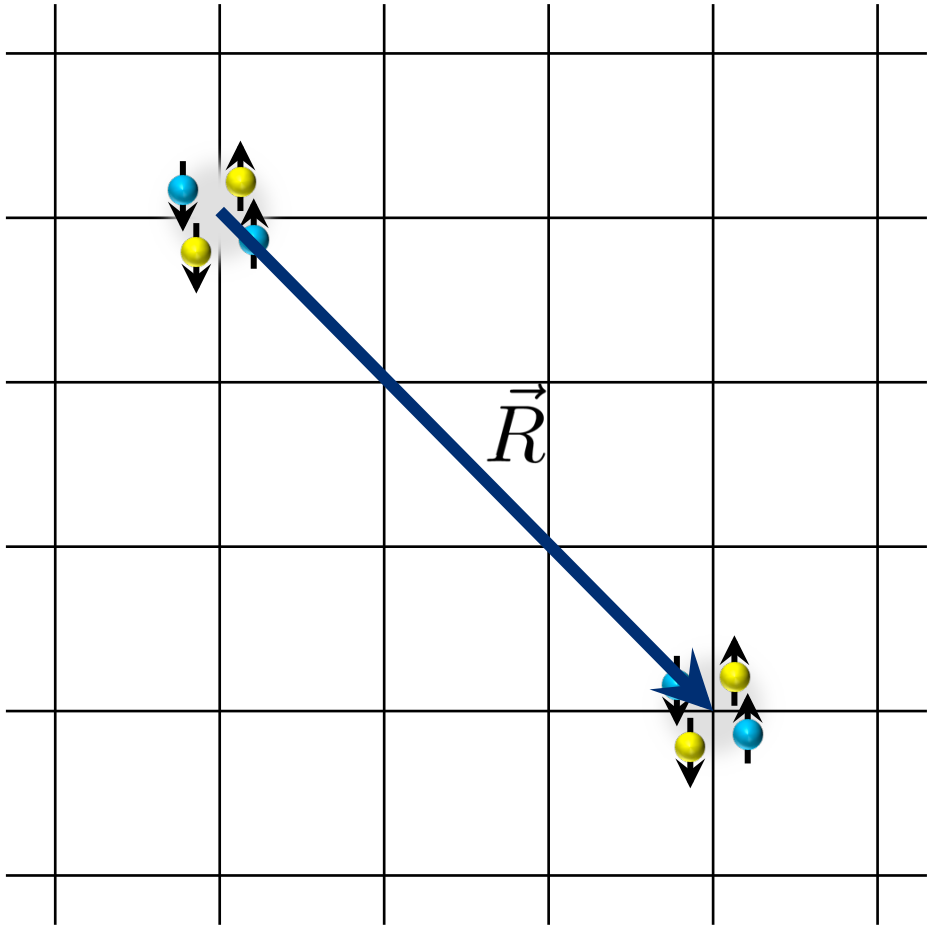
Strategy is to divide the problem into two parts. In the first part, we use Euclidean time projection and lattice Monte Carlo to derive an *ab initio* low-energy cluster Hamiltonian, called the adiabatic Hamiltonian.

In the second part, we use the adiabatic Hamiltonian to compute scattering phase shifts or reaction amplitudes.

Computational scaling is roughly quadratic in the number of nucleons.

Start with localized cluster states for all possible separation vectors $\vec{R}$

$$|\vec{R}\rangle = \sum_{\vec{r}} |\vec{r}+\vec{R}\rangle_1 \otimes |\vec{r}\rangle_2$$



Use projection Monte Carlo to propagate cluster wave functions in Euclidean time to form dressed cluster states

$$|\vec{R}\rangle_\tau = \exp(-H\tau)|\vec{R}\rangle$$

We then evaluate matrix elements of the full microscopic Hamiltonian with respect to the dressed cluster states,

$$[H_\tau]_{\vec{R},\vec{R}'} = {}_\tau\langle\vec{R}|H|\vec{R}'\rangle_\tau$$

Since the dressed cluster states are in general not orthogonal, we construct a norm matrix given by the inner product

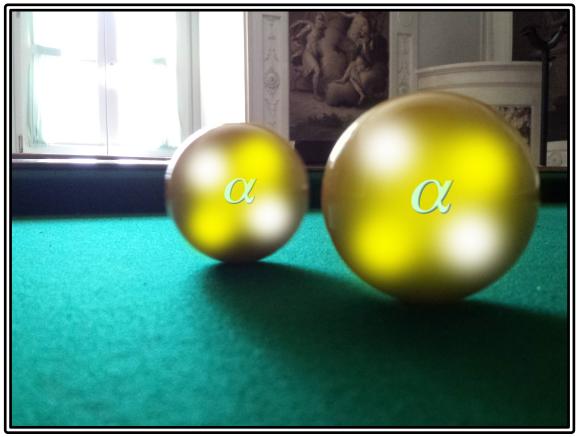
$$[N_\tau]_{\vec{R},\vec{R}'} = {}_\tau\langle\vec{R}|\vec{R}'\rangle_\tau$$

The adiabatic Hamiltonian is defined by the matrix product

$$[H^a_\tau]_{\vec{R},\vec{R}'} = \left[N_\tau^{-1/2} H_\tau N_\tau^{-1/2}\right]_{\vec{R},\vec{R}'}$$

We now treat the adiabatic Hamiltonian as an effective two-particle Hamiltonian for scattering and reaction calculations.

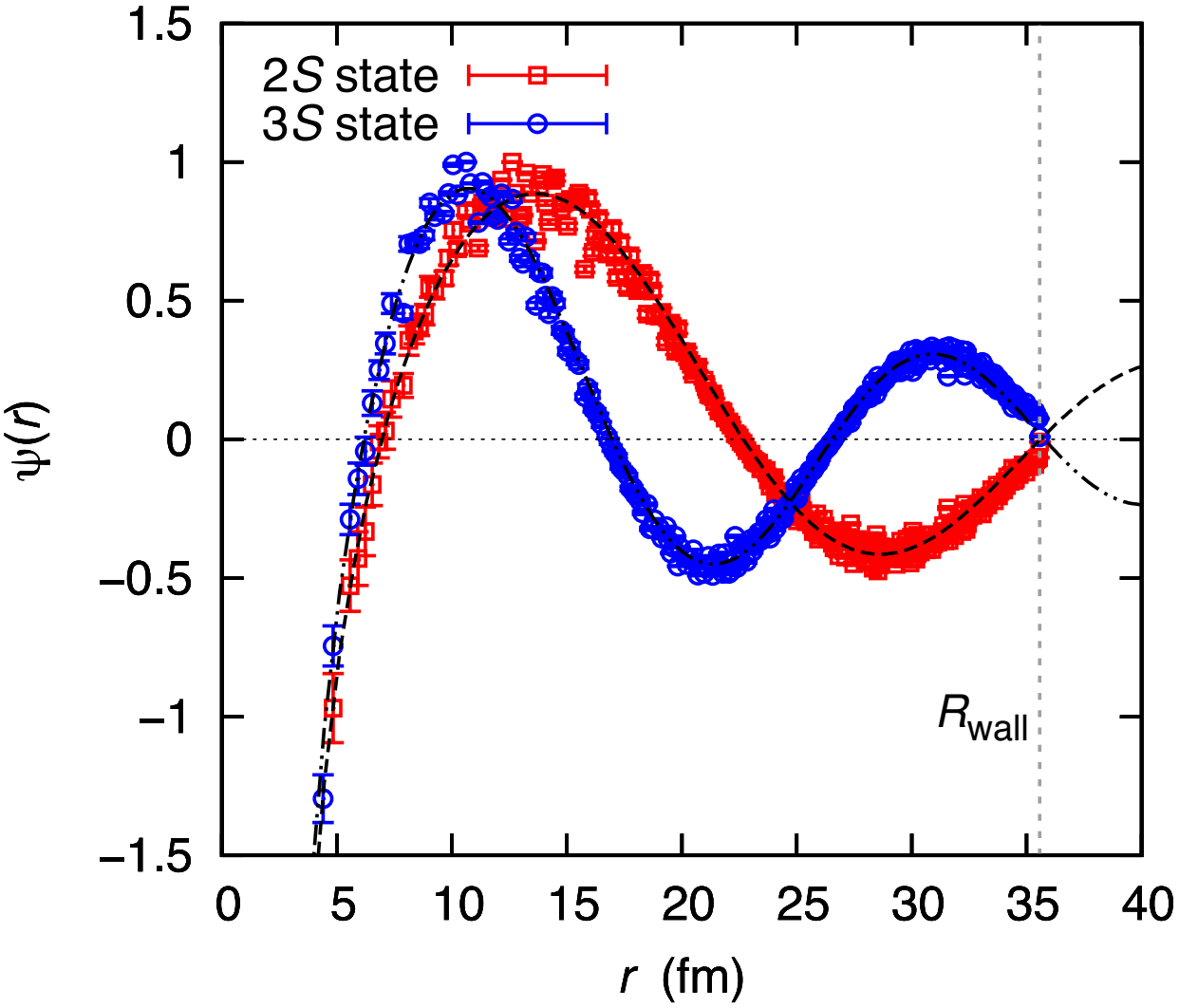
$$^4\mathrm{He} + {}^4\mathrm{He} \rightarrow {}^4\mathrm{He} + {}^4\mathrm{He}$$



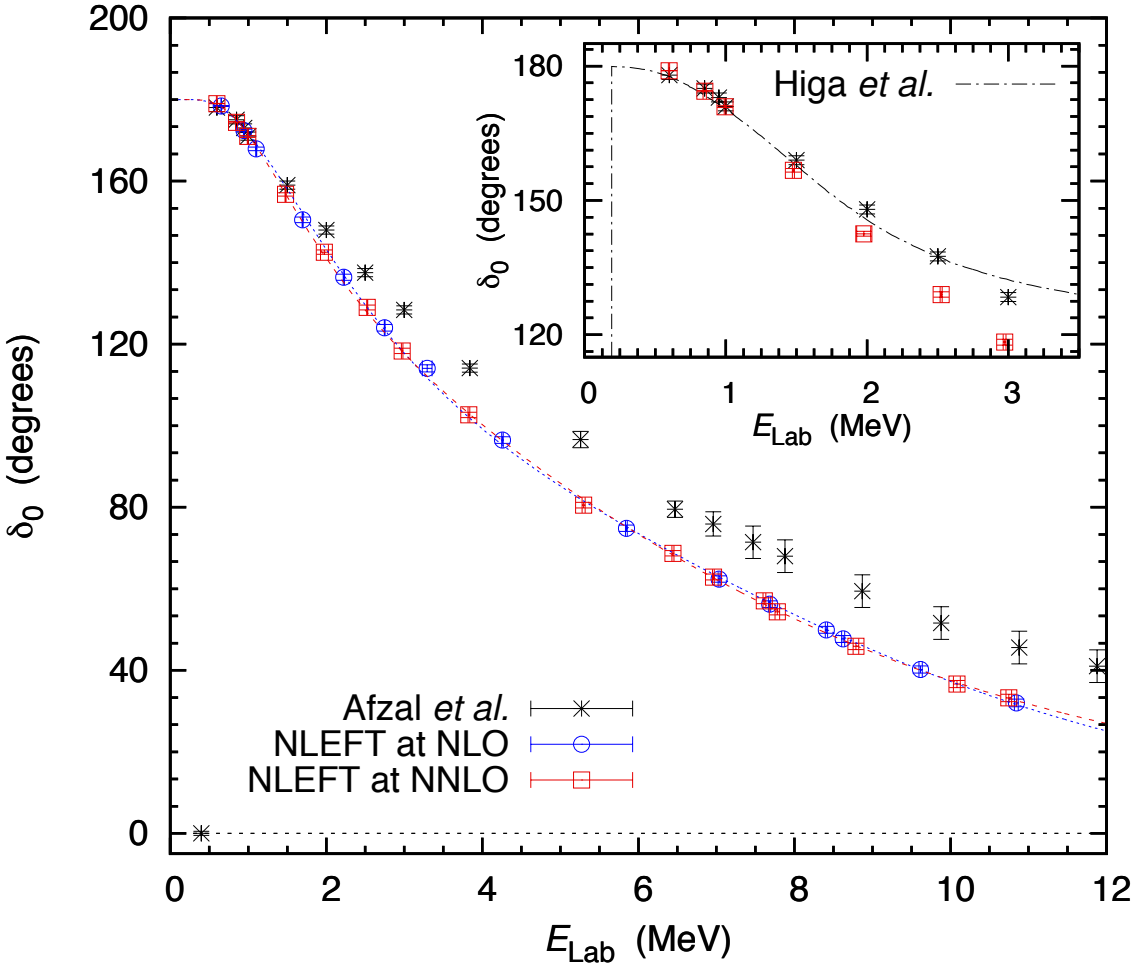
Ab initio results for alpha-alpha scattering up to NNLO with lattice spacing 1.97 fm.

Using the adiabatic projection method, we performed lattice simulations for the *S*-wave and *D*-wave channels.

Elhatisari, D.L., Rupak, Epelbaum, Krebs, Lähde, Luu, Meißner, Nature 528, 111 (2015)


2S state
3S state
1.5
1
0.5
0
−0.5
−1
−1.5
ψ(r)
0
5
10
15
20
25
30
35
40
r (fm)
R_wall

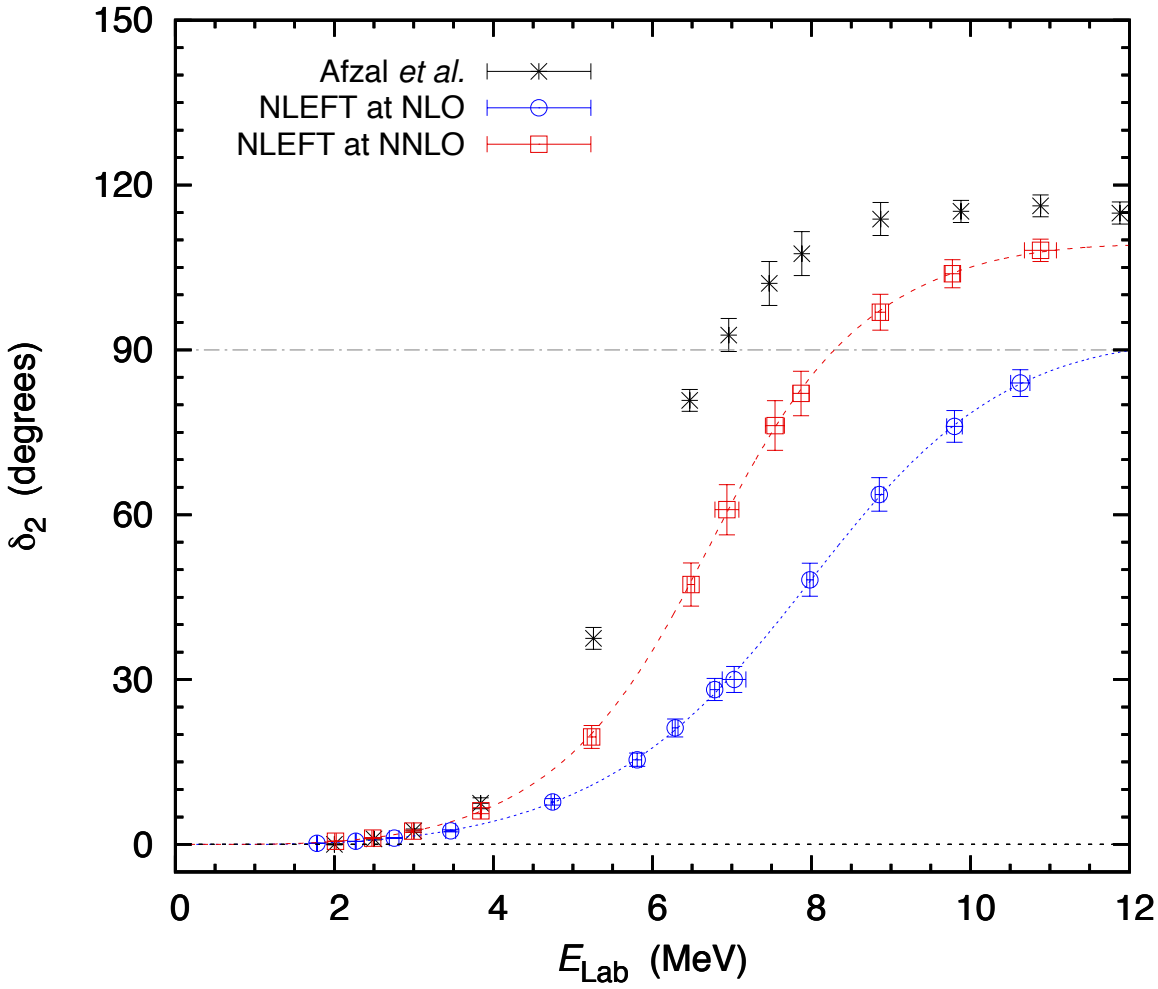
$^4\mathrm{He} + {}^4\mathrm{He} \rightarrow {}^4\mathrm{He} + {}^4\mathrm{He}$



Afzal, Ahmad, Ali, RMP 41 247 (1969)

Higa, Hammer, van Kolck, NPA 809 171(2008)

$^4\mathrm{He} + {}^4\mathrm{He} \rightarrow {}^4\mathrm{He} + {}^4\mathrm{He}$



Challenge

There has been no algorithm available for *ab initio* auxiliary field Monte Carlo simulations to determine the density distribution of particles relative to the center of mass. The problem is that the particle wave functions in the auxiliary field simulation are a superposition of many values for the center of mass.

Pinhole algorithm

Consider the density operator for nucleon with spin i and isospin j

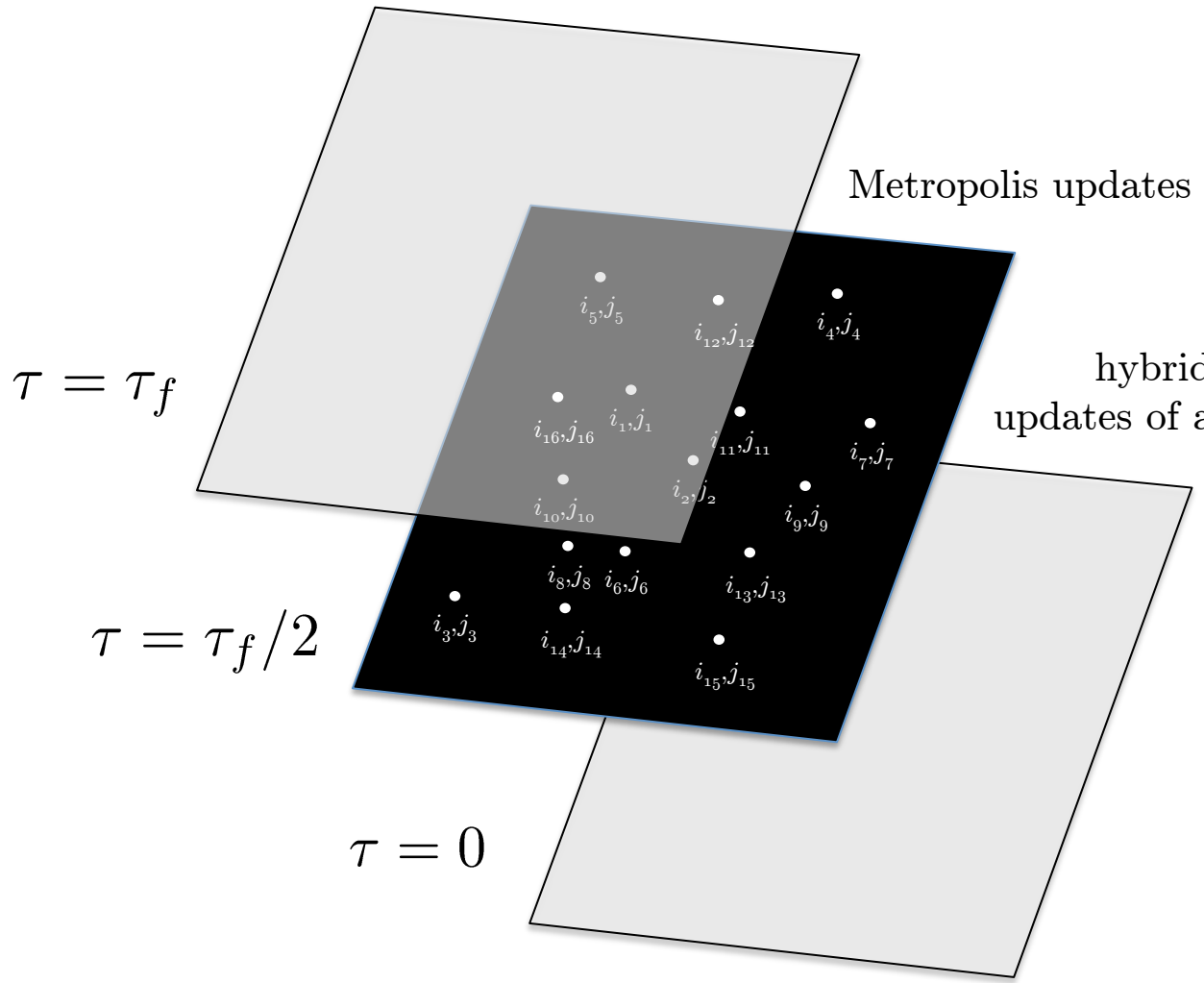
$$\rho_{i,j}(\mathbf{n}) = a^{\dagger}_{i,j}(\mathbf{n}) a_{i,j}(\mathbf{n})$$

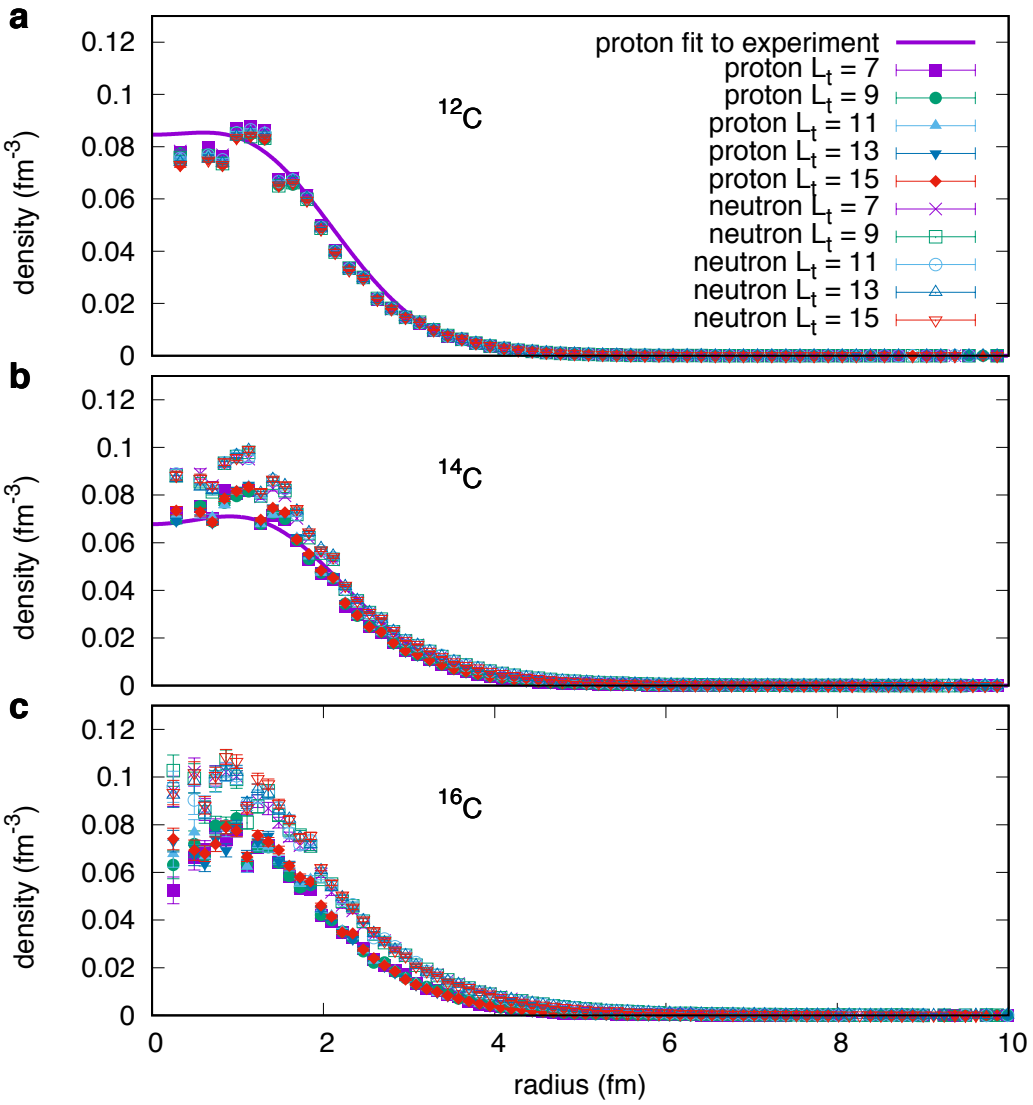
We construct the normal-ordered A-body density operator

$$\rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A) = :\rho_{i_1,j_1}(\mathbf{n}_1)\cdots\rho_{i_A,j_A}(\mathbf{n}_A):$$

In the simulations we do Monte Carlo sampling of the amplitude

$$A_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A,t) = \langle\Psi_I|e^{-Ht/2}\rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A)e^{-Ht/2}|\Psi_I\rangle$$

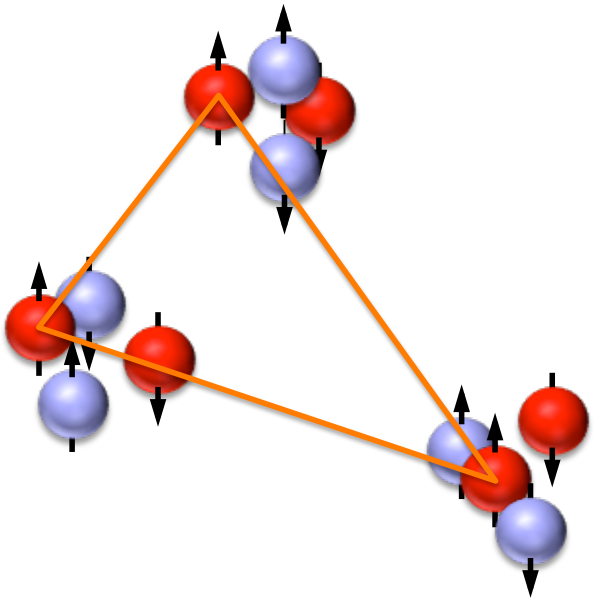

Metropolis updates of pinholes
hybrid Monte Carlo
updates of auxiliary/pion fields
$\tau = \tau_f$
$\tau = \tau_f/2$
$\tau = 0$
i_5,j_5
i_{12},j_{12}
i_4,j_4
i_{16},j_{16}
i_1,j_1
i_{11},j_{11}
i_7,j_7
i_2,j_2
i_{10},j_{10}
i_9,j_9
i_8,j_8
i_6,j_6
i_{13},j_{13}
i_3,j_3
i_{14},j_{14}
i_{15},j_{15}



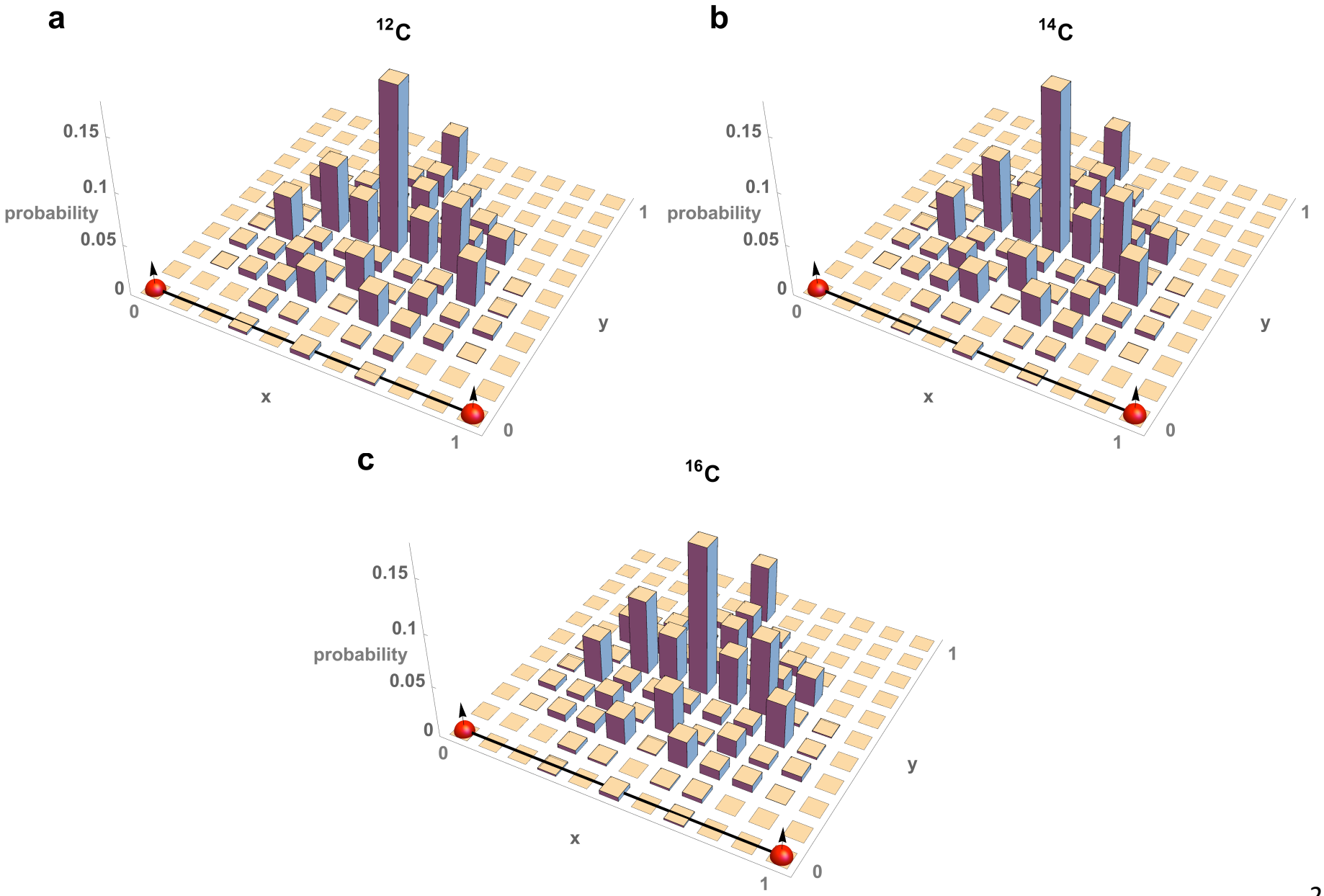
Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, PRL 119, 222505 (2017)

Model-independent measure of alpha cluster geometry

For the carbon isotopes, we can map out the alpha cluster geometry by computing the density correlations of the three spin-up protons. We compute these density correlations using the pinhole algorithm.



Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, PRL 119, 222505 (2017)


a
^{12}C
0.15
0.1
probability
0.05
0
0
x
1
0
y
1
b
^{14}C
0.15
0.1
probability
0.05
0
0
x
1
0
y
1
c
^{16}C
0.15
0.1
probability
0.05
0
0
x
1
0
y
1

Challenge

In order to compute thermodynamic properties of finite nuclei, nuclear matter, and neutron matter, we need to compute the partition function

$$\mathrm{Tr}\exp(-\beta H)$$

The standard method for computing the partition function involves calculating determinants of matrices of size $4V \times 4V$, where V is the number of lattice points filling the spatial volume. Since V is usually several hundred or several thousand, these calculations are very expensive.

Pinhole trace algorithm

We have developed an alternative method using pinholes that calculates determinants of matrices of size $A \times A$, where A is the number of nucleons. The method does not suffer from severe sign oscillations.

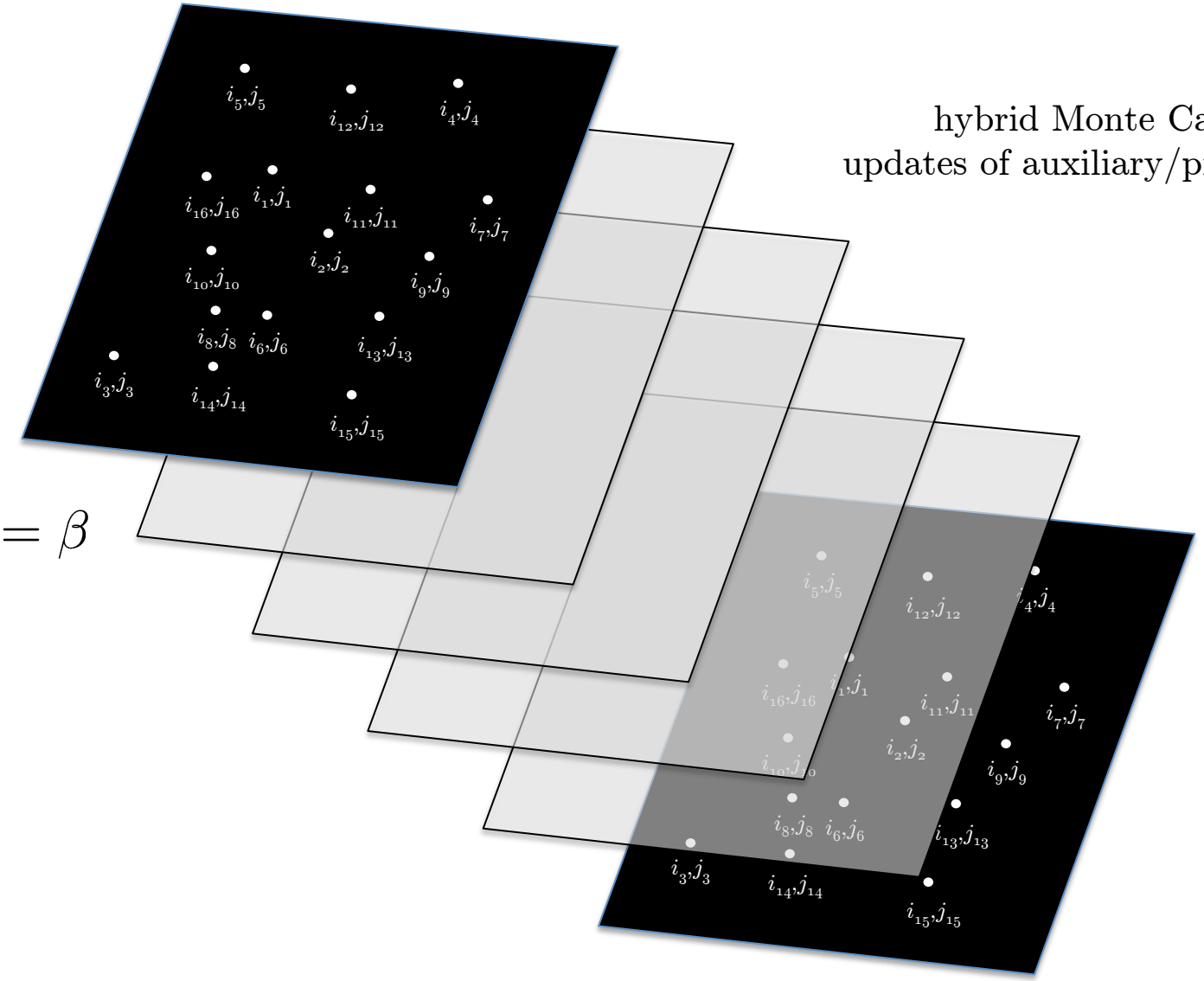
We compute the quantum mechanical trace over A-nucleon states by summing over pinholes (position eigenstates) for the initial and final states

$$\mathrm{Tr}\, O = \frac{1}{A!} \sum_{i_1 \cdots i_A, j_1 \cdots j_A, \mathbf{n}_1 \cdots \mathbf{n}_A} \langle 0 | a_{i_A, j_A}(\mathbf{n}_A) \cdots a_{i_1, j_1}(\mathbf{n}_1)\, O\, a^\dagger_{i_1, j_1}(\mathbf{n}_1) \cdots a^\dagger_{i_A, j_A}(\mathbf{n}_A) | 0 \rangle$$

This can be used to calculate the partition function in the canonical ensemble.

Work in progress. B. Lu, *et al.*

Metropolis updates of pinholes



hybrid Monte Carlo
updates of auxiliary/pion fields

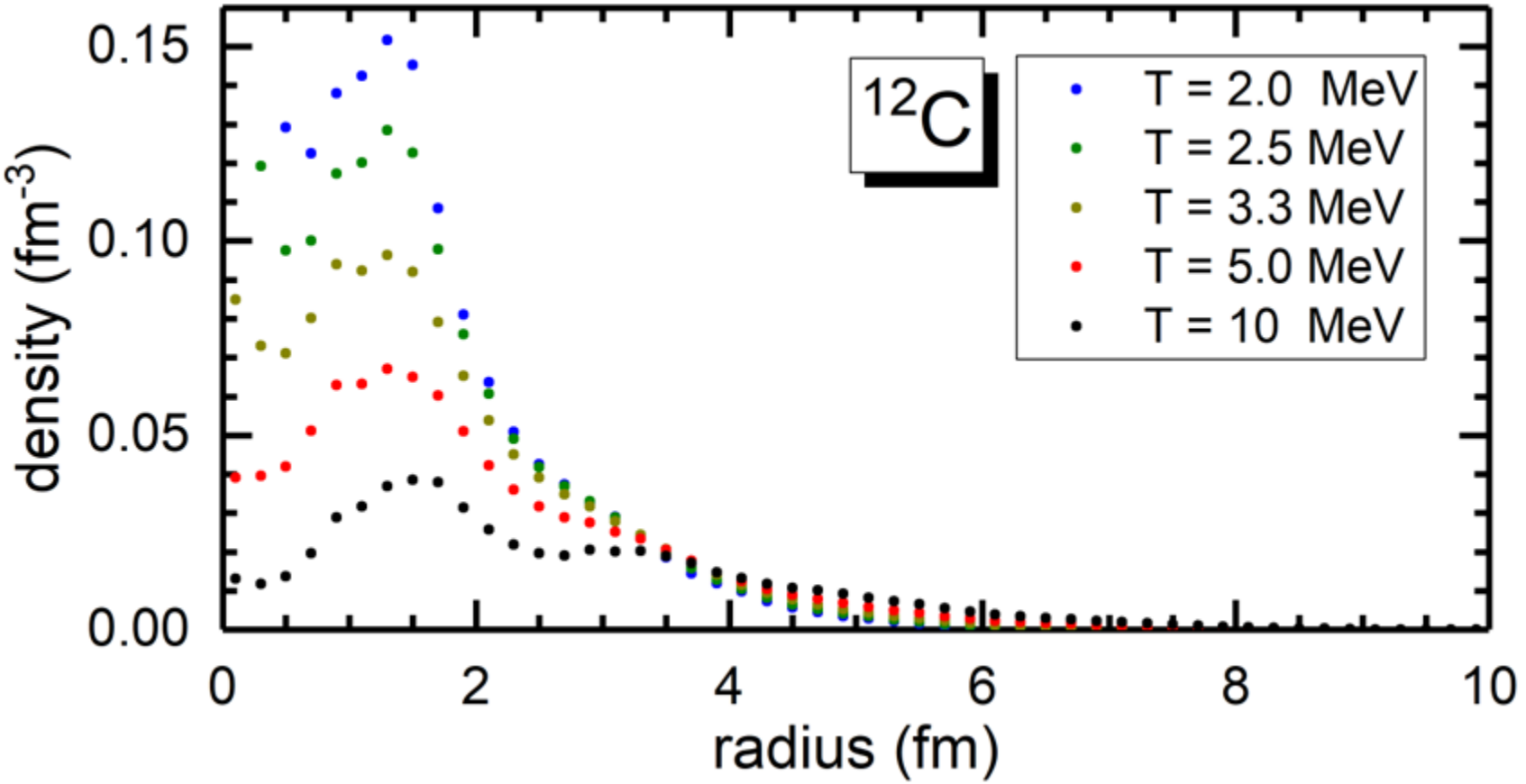


Figure courtesy of Bingnan Lu

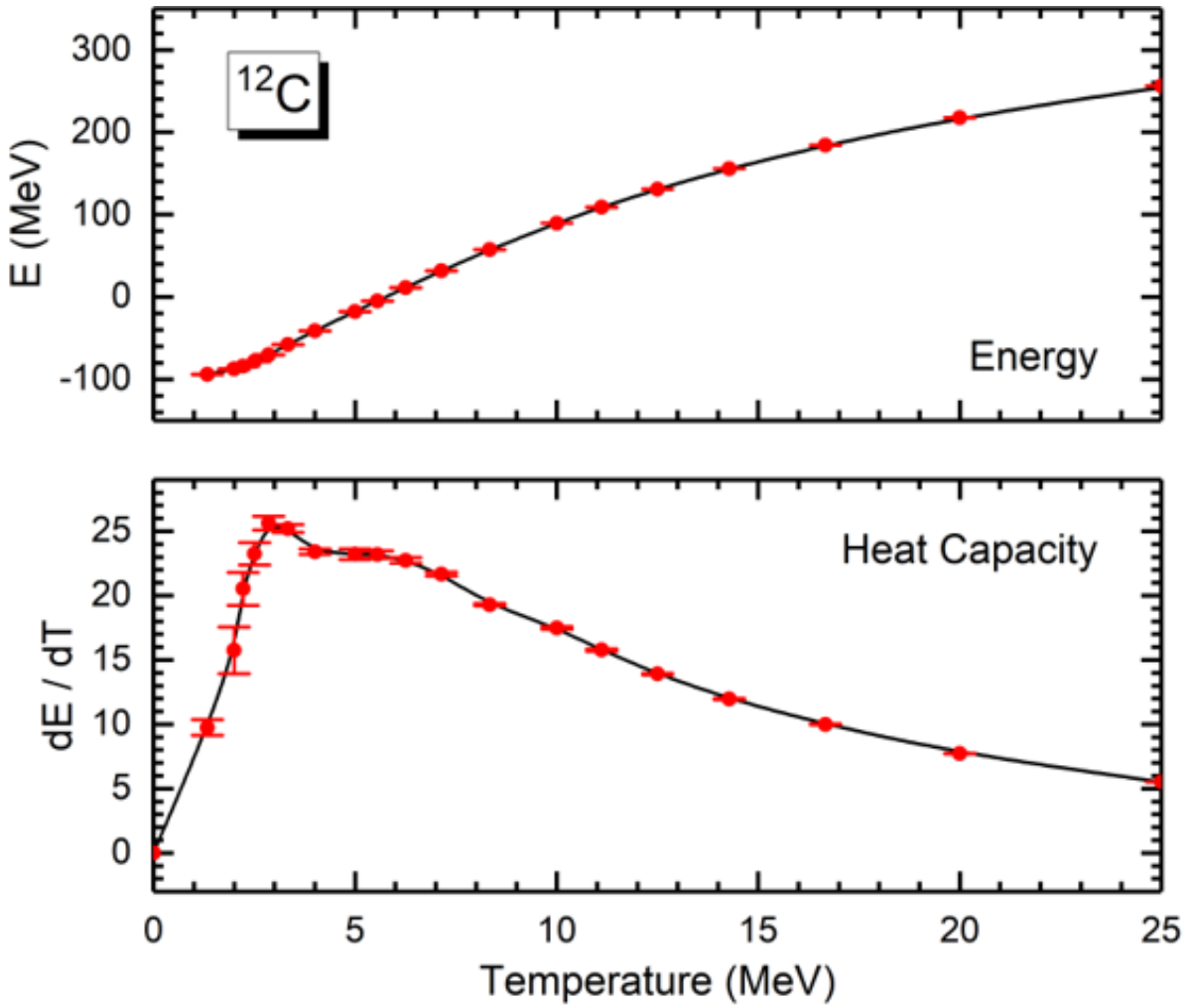


Figure courtesy of Bingnan Lu

Challenge

A common challenge faced in many fields of quantum physics is finding the extremal eigenvalues and eigenvectors of a Hamiltonian matrix too large to store in computer memory.

There are numerous efficient methods developed for this task. All existing methods either use Monte Carlo simulations, diagrammatic expansions, variational methods, or some combination.

The problem is that they generally fail when some control parameter in the Hamiltonian matrix exceeds some threshold value.

Eigenvector continuation

We demonstrate that when a control parameter in the Hamiltonian matrix is varied smoothly, the extremal eigenvectors do not explore the large dimensionality of the linear space. Instead they trace out trajectories with significant displacements in only a small number of linearly-independent directions.

We prove this empirical observation using analytic function theory and the principles of analytic continuation.

Since the eigenvector trajectory is a low-dimensional manifold embedded in a very large space, we can find the desired eigenvector using methods similar to image recognition in machine learning.

D. Frame, R. He, I. Ipsen, Da. Lee, De. Lee, E. Rrapaj, arXiv:1711.07090

Consider a one-parameter family of Hamiltonian matrices of the form

$$H(c) = H_0 + cH_1$$

where H_0 and H_1 are Hermitian. Let the eigenvalues and eigenvectors be

$$H(c)|\psi_j(c)\rangle = E_j(c)|\psi_j(c)\rangle$$

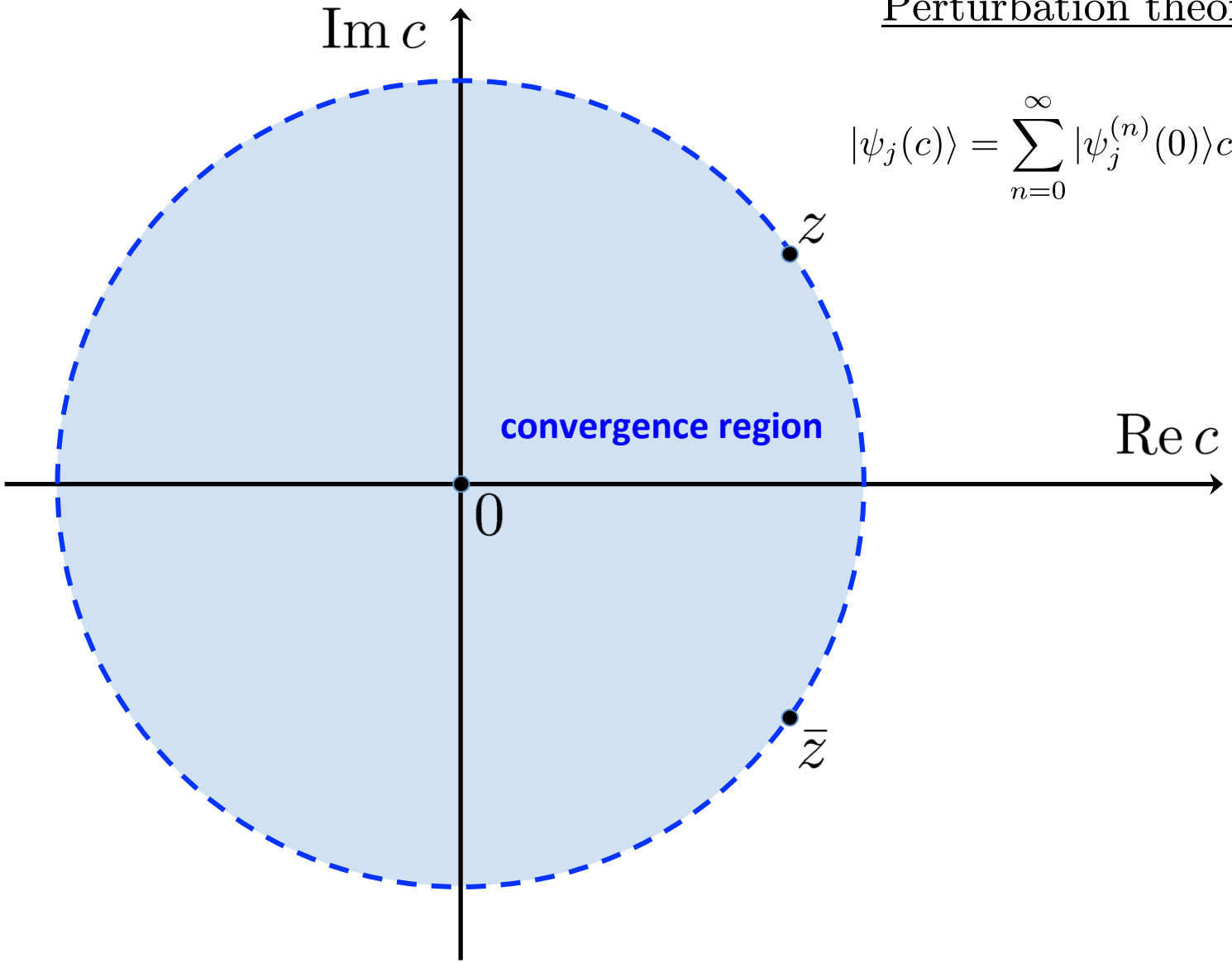
We can perform series expansions around the point $c = 0$.

$$E_j(c) = \sum_{n=0}^{\infty} E_j^{(n)}(0)c^n/n!$$
$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(0)\rangle c^n/n!$$

This is the strategy of perturbation theory. We can compute each term in the series when the eigenvalues and eigenvectors of H_0 are known or computable.

Perturbation theory

$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(0)\rangle c^n/n!$$



Bose-Hubbard model

In order to illuminate our discussion with a concrete example, we consider a quantum Hamiltonian known as the Bose-Hubbard model in three dimensions. It describes a system of identical bosons on a three-dimensional cubic lattice.

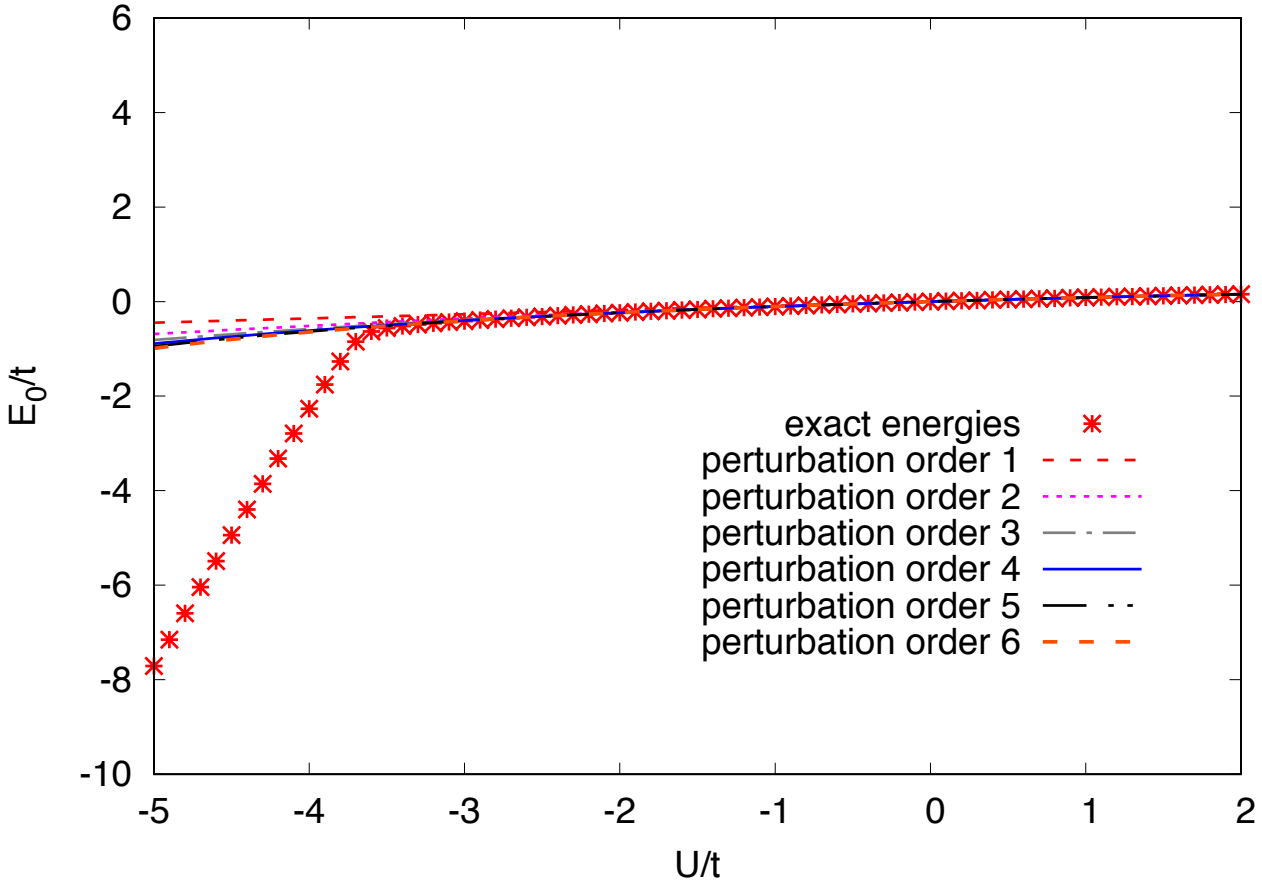
$$H = -t \sum_{\langle \mathbf{n}', \mathbf{n} \rangle} a^\dagger(\mathbf{n}') a(\mathbf{n}) + \frac{U}{2} \sum_{\mathbf{n}} \rho(\mathbf{n})[\rho(\mathbf{n}) - \mathbf{1}] - \mu \sum_{\mathbf{n}} \rho(\mathbf{n})$$

$$\rho(\mathbf{n}) = a^\dagger(\mathbf{n}) a(\mathbf{n})$$

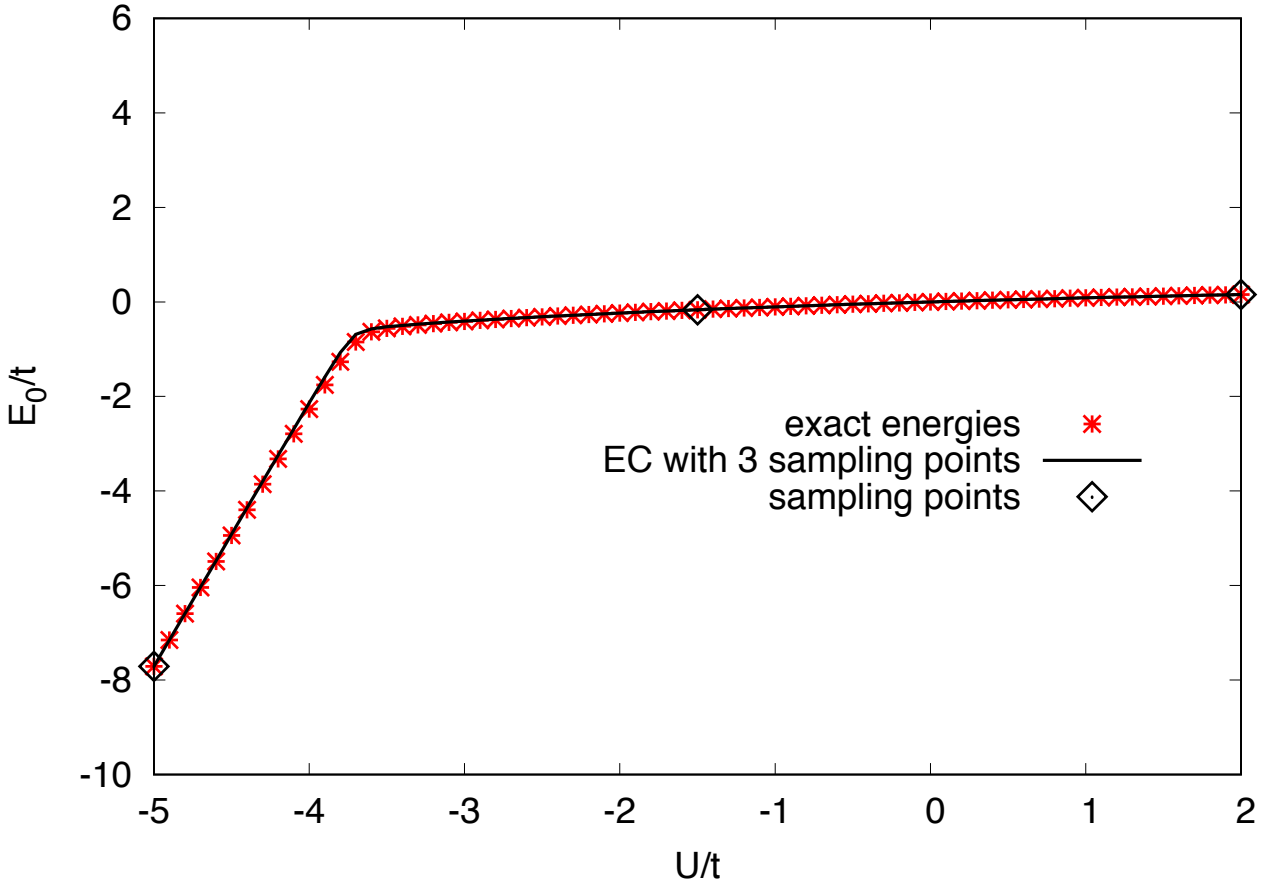
The parameter t controls the hopping the bosons on the lattice, and U is the single-site pairwise interaction. We set the chemical potential to be

$$\mu = -6t$$

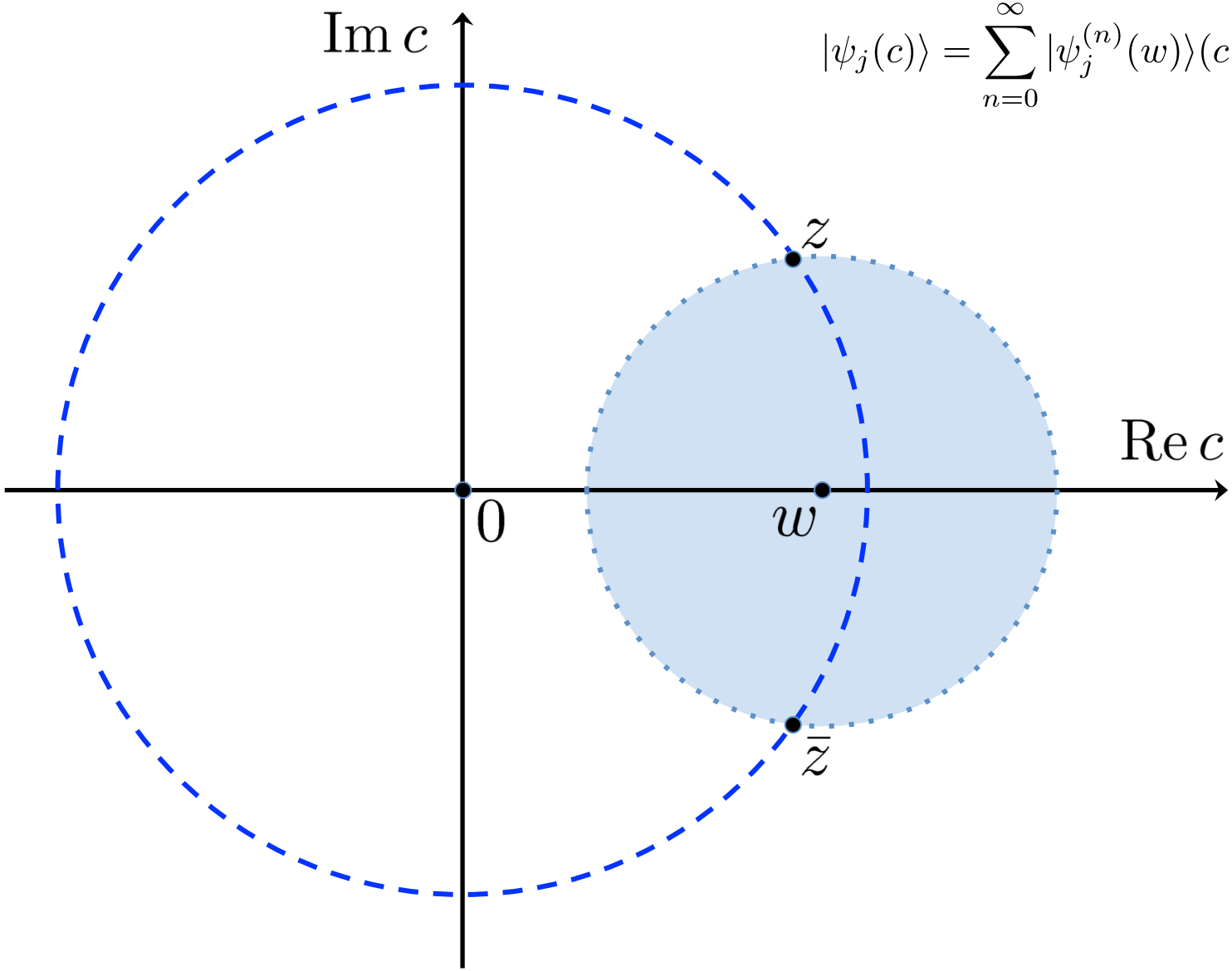
Perturbation theory fails at strong attractive coupling

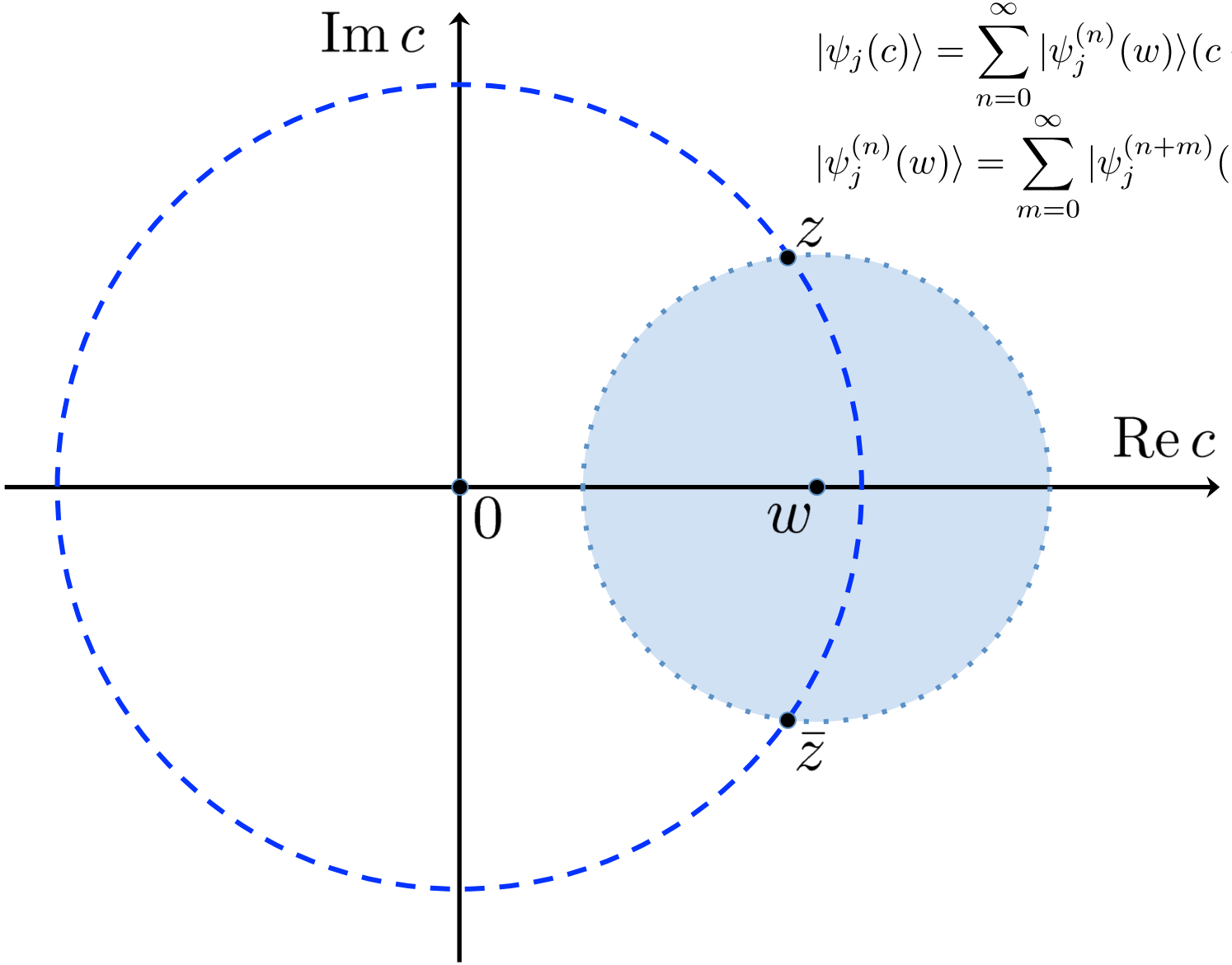


Restrict the linear space to the span of three vectors



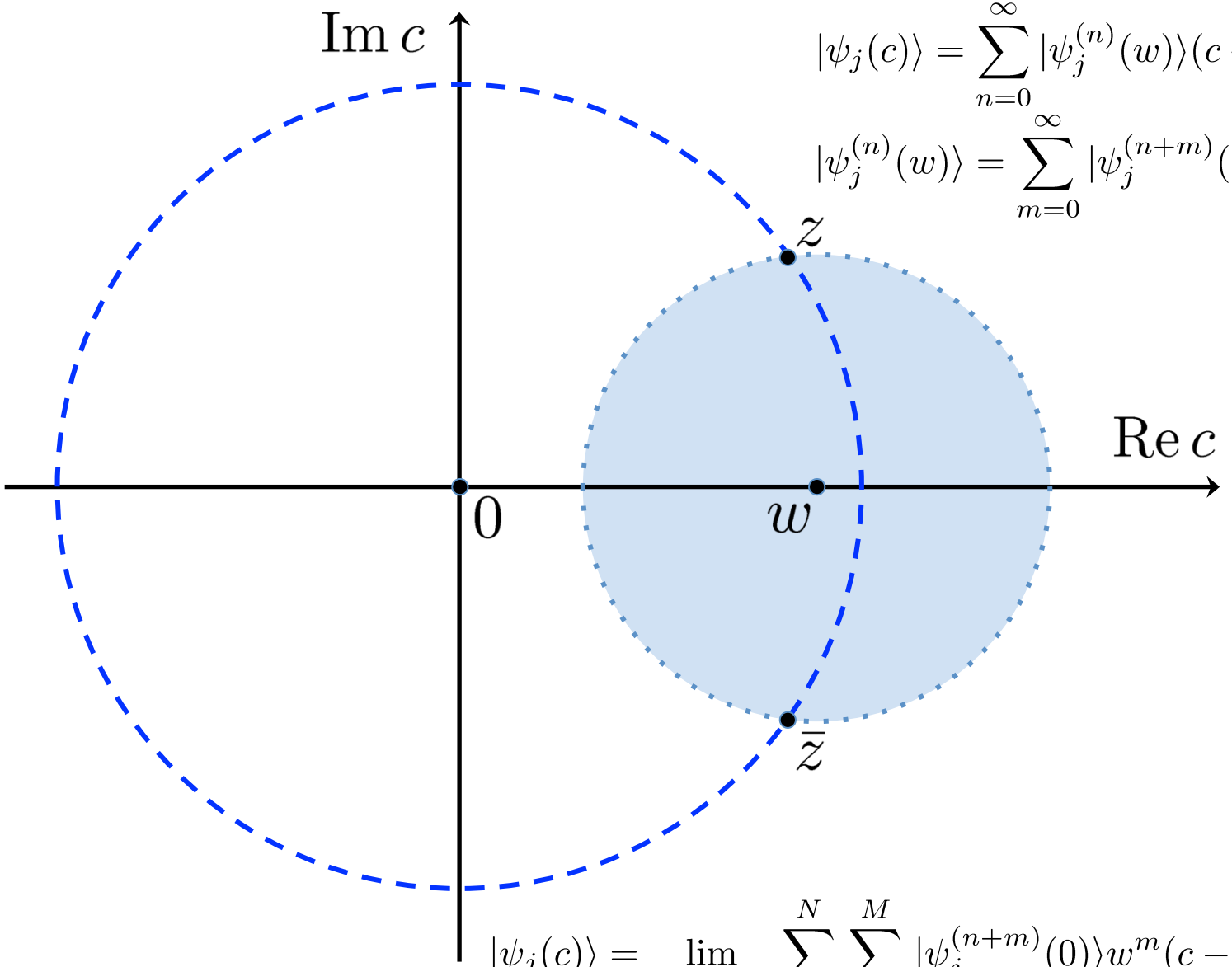
$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(w)\rangle (c-w)^n/n!$$





$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(w)\rangle (c-w)^n/n!$$

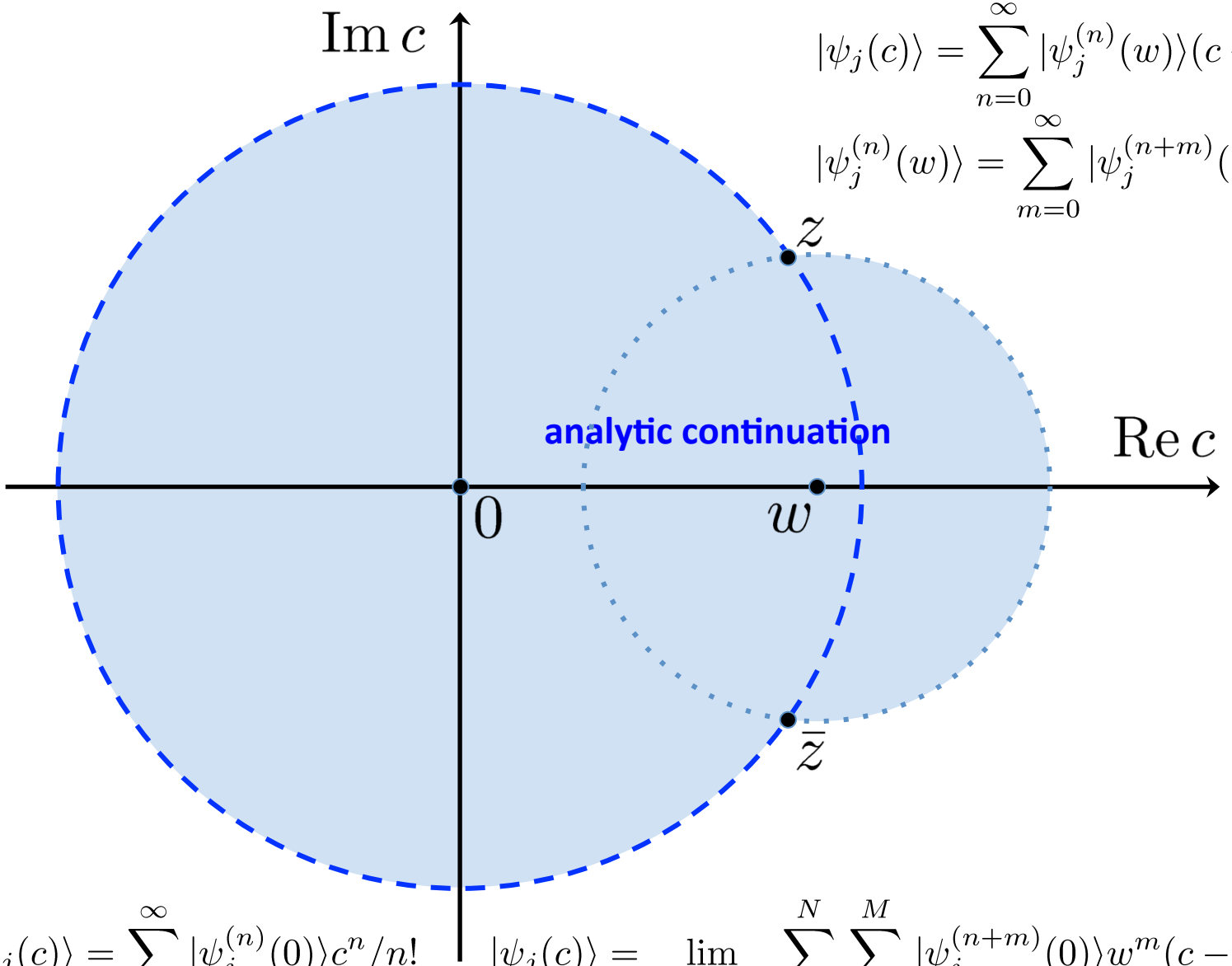
$$|\psi_j^{(n)}(w)\rangle = \sum_{m=0}^{\infty} |\psi_j^{(n+m)}(0)\rangle w^m/m!$$



$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(w)\rangle (c-w)^n/n!$$

$$|\psi_j^{(n)}(w)\rangle = \sum_{m=0}^{\infty} |\psi_j^{(n+m)}(0)\rangle w^m/m!$$

$$|\psi_j(c)\rangle = \lim_{N,M\to\infty} \sum_{n=0}^{N}\sum_{m=0}^{M} |\psi_j^{(n+m)}(0)\rangle w^m (c-w)^n/(m!\,n!)$$



$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(w)\rangle (c-w)^n/n!$$

$$|\psi_j^{(n)}(w)\rangle = \sum_{m=0}^{\infty} |\psi_j^{(n+m)}(0)\rangle w^m/m!$$

$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(0)\rangle c^n/n!$$

$$|\psi_j(c)\rangle = \lim_{N,M\to\infty} \sum_{n=0}^{N} \sum_{m=0}^{M} |\psi_j^{(n+m)}(0)\rangle w^m (c-w)^n/(m!\,n!)$$

The eigenvector can be well approximated as a linear combination of a few vectors, using either the original series expansion

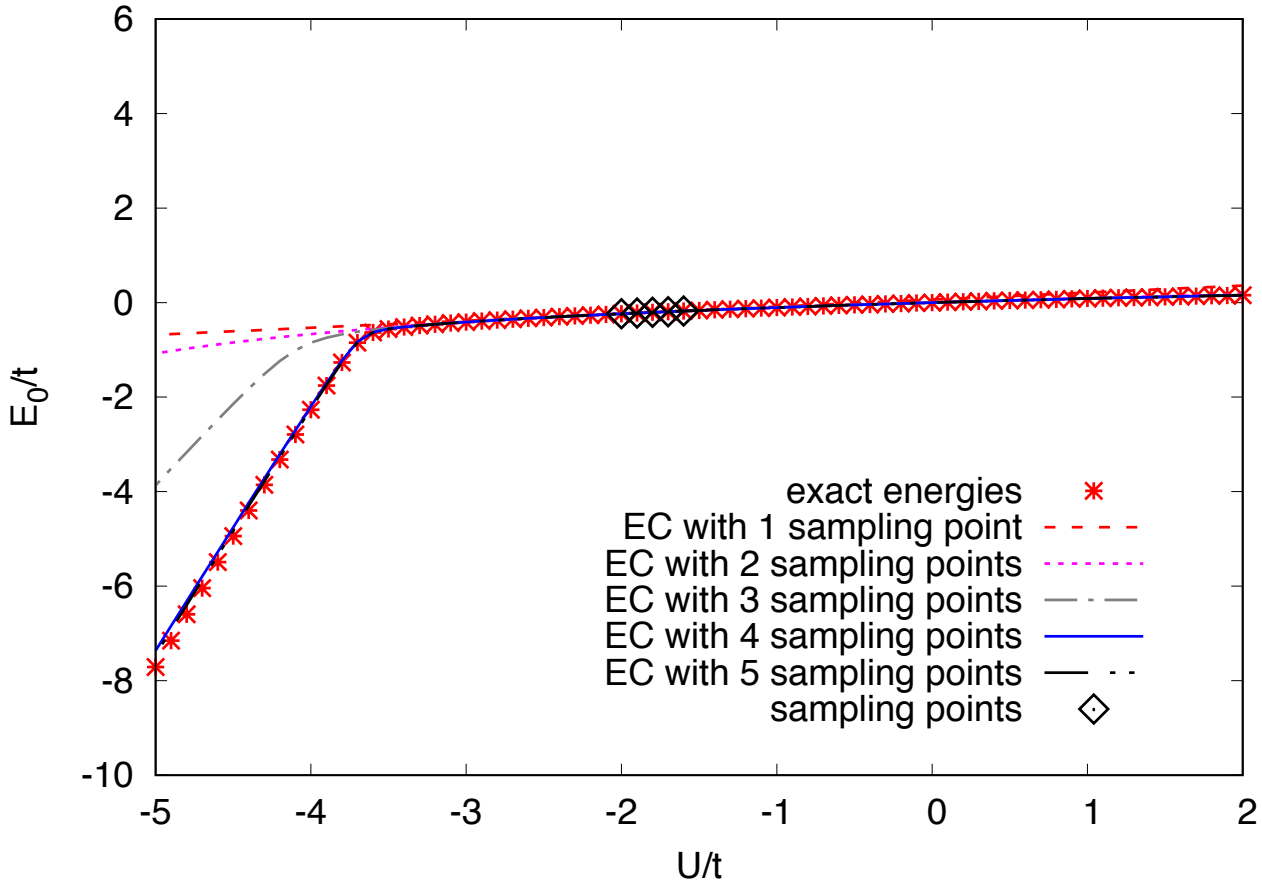
$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(0)\rangle c^n/n!$$

or the rearranged multi-series expansion we obtained through analytic continuation

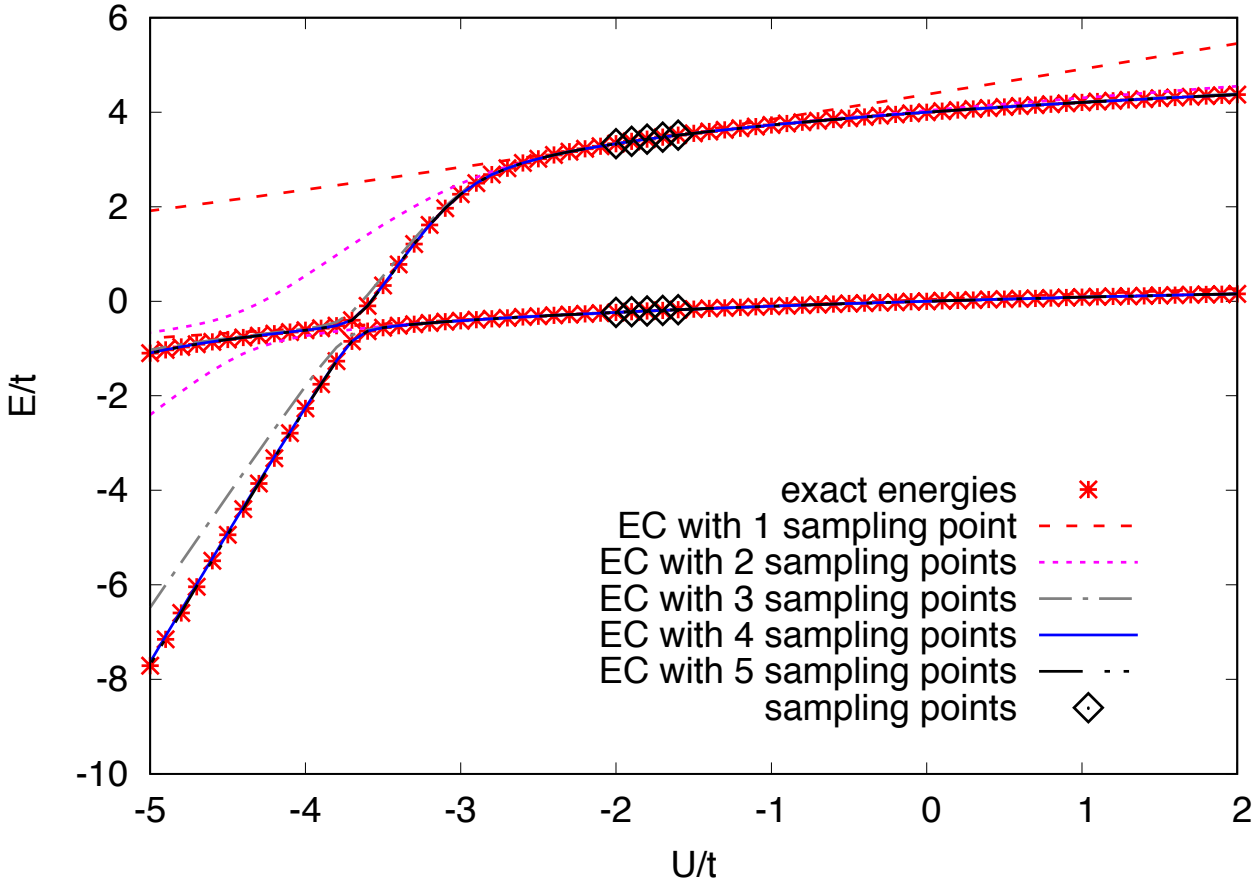
$$|\psi_j(c)\rangle = \lim_{N,M\to\infty} \sum_{n=0}^{N} \sum_{m=0}^{M} |\psi_j^{(n+m)}(0)\rangle w^m (c-w)^n/(m!\,n!)$$

As c is varied the eigenvector does not explore the large dimensionality of the linear space, but is instead well approximated by a low-dimension manifold.

We can "learn" the eigenvector trajectory in one region and perform eigenvector continuation to another region

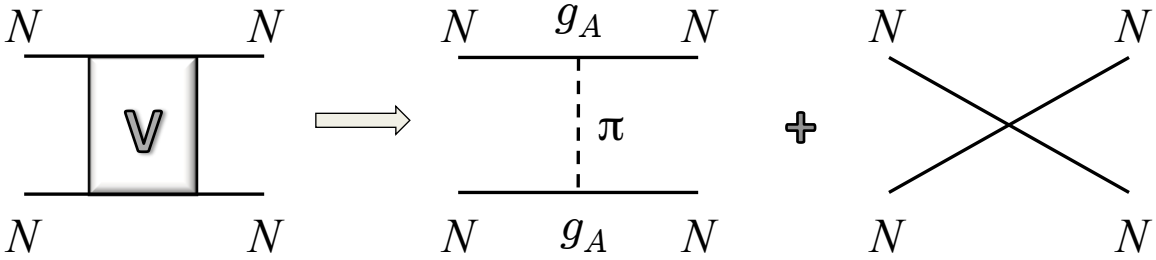


Applying eigenvector continuation to more than one eigenvector at a time accelerates convergence near avoided level crossings.



Application: Neutron matter simulations

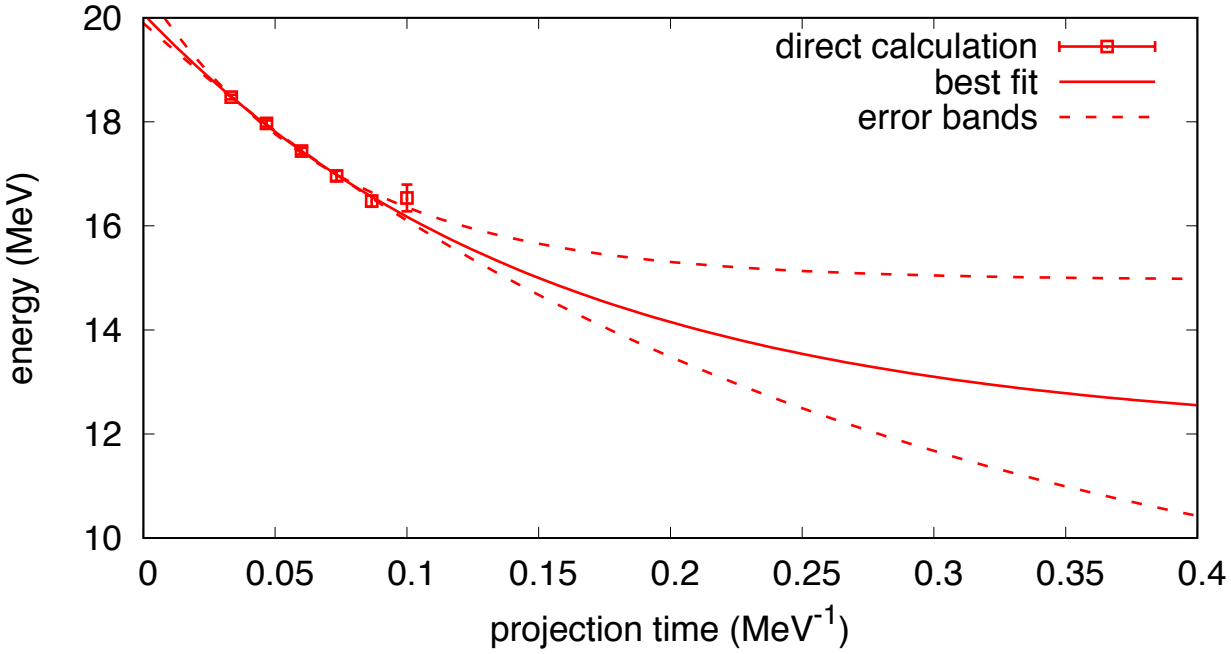
We consider lattice effective field theory simulations of the neutron matter at the leading order.



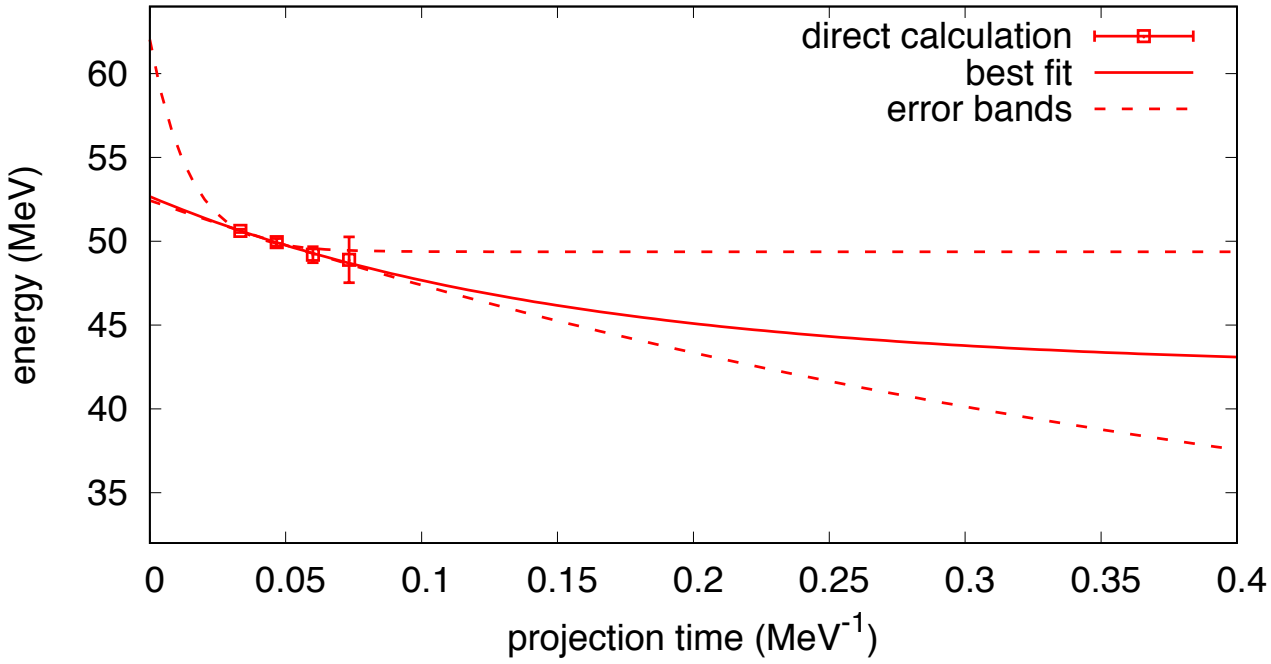
As a challenge to the eigenvector continuation technique, we use a lattice action for one-pion exchange that causes severe Monte Carlo sign oscillations.

D.L., in "An Advanced Course in Computational Nuclear Physics", Hjorth-Jensen, Lombardo, van Kolck, Eds., Lecture Notes in Physics, Volume 936 [arXiv:1609.00421]

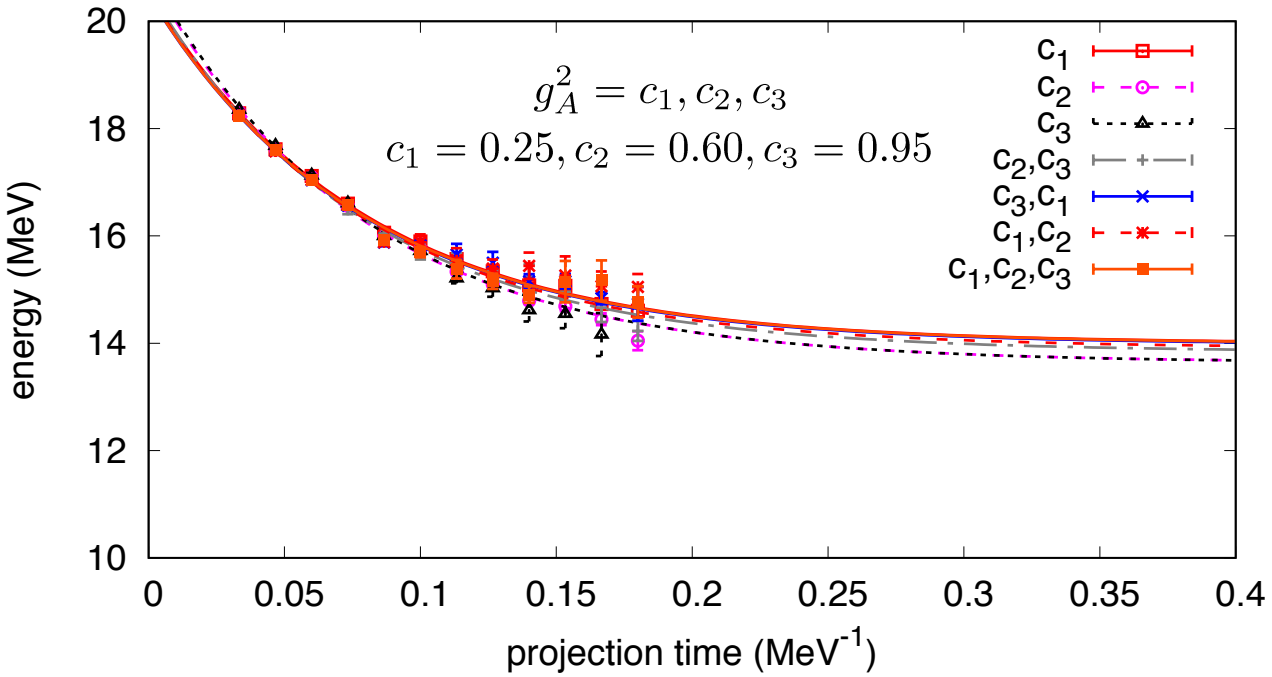
Direct calculation of six neutrons ($L = 8$ fm)



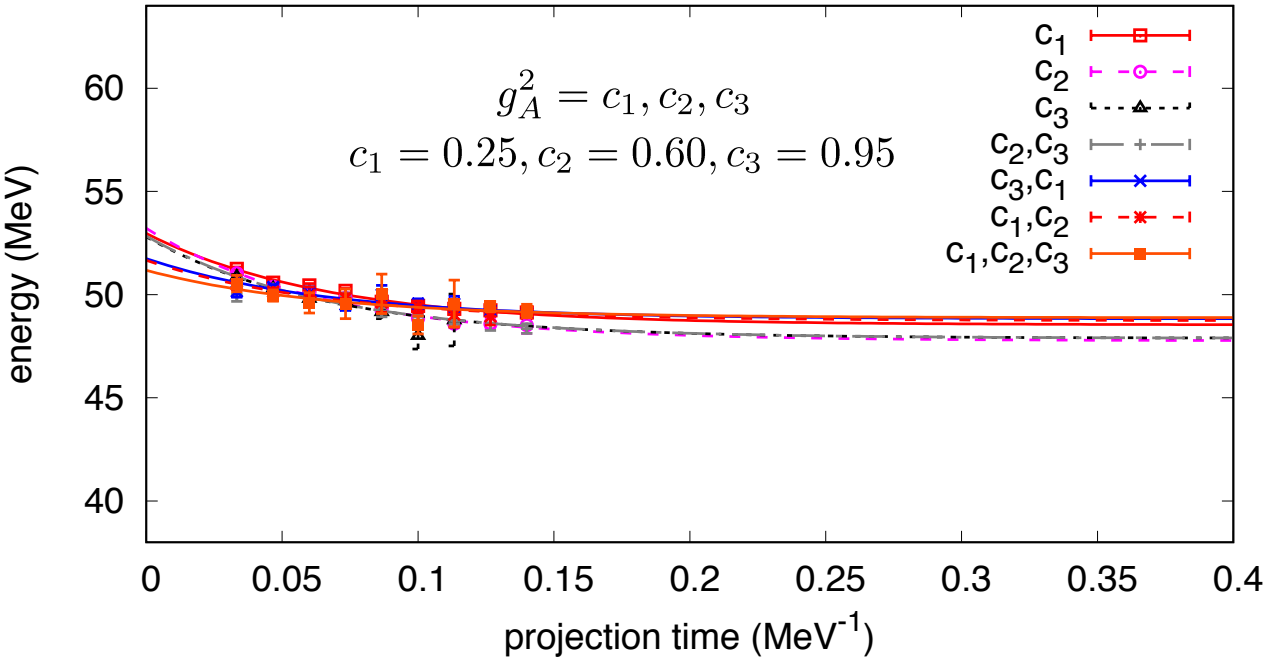
Direct calculation of fourteen neutrons ($L = 8$ fm)



Eigenvector continuation for six neutrons ($L = 8$ fm)



Eigenvector continuation for fourteen neutrons ($L = 8$ fm)



g_A^2 values	E_0 for six neutrons (MeV)	E_0 for fourteen neutrons (MeV)
c_1	13.8(1)	48.9(4)
c_2	13.6(2)	48.4(5)
c_3	13.6(2)	48.9(6)
c_2, c_3	13.6(2)	48.1(6)
c_3, c_1	13.6(2)	48.9(6)
c_1, c_2	13.6(2)	48.0(6)
c_1, c_2, c_3	13.6(2)	48.0(6)
direct calculation	$12(^{+3}_{-4})$	$42(^{+7}_{-15})$

Summary and Outlook

These are exciting times for the *ab initio* nuclear theory community. In lattice EFT, we have new projects in motion which are pushing the current frontiers.

Currently working to improve our understanding of the detailed connection between bare nuclear forces and nuclear structure for light and medium-mass nuclei.

Applying the adiabatic projection method to low-energy nucleon-nucleus and alpha-nucleus scattering and reactions.

Using the pinhole algorithm to study the detailed structure of nuclei and thermodynamics of finite nuclei, nuclear matter, and neutron matter.

Implementing eigenvector continuation to treat all higher-order interactions in chiral effective field theory.